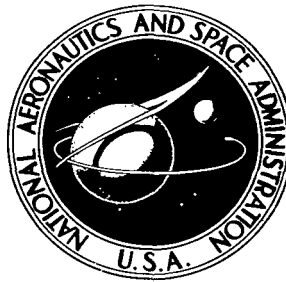


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SIMPLIFIED METHODS FOR CALCULATING  
PHOTODISSOCIATION RATES OF VARIOUS  
MOLECULES IN SCHUMANN-RUNGE BAND  
SYSTEMS IN THE UPPER ATMOSPHERE

*Tatsuo Shimazaki, Toshihiro Ogawa,  
and B. C. Farrell*

*Ames Research Center  
Moffett Field, Calif. 94035*



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Tatsuo Shimazaki, Toshihiro Ogawa,\* and B. C. Farrell\*\*

Ames Research Center

SUMMARY

Simplified methods proposed by Hudson and Mahle, and Kockarts for calculating the transmission of solar UV radiation and the dissociation coefficients of various molecules in the Schumann-Runge band spectral region are compared. A significant difference sometimes appears in calculations of the individual band, but the total transmission and the total dissociation coefficients integrated over the entire SR band region agree well between the two methods. The ambiguities in the solar flux data affect the calculated dissociation coefficients more strongly than does the method. A simpler method is developed for the purpose reducing the computation time and computer memory size necessary for storing coefficients of the equations. The new method can reduce the computation time by a factor of more than 3 and the memory size by a factor of more than 50 compared with the Hudson-Mahle method, and yet the result agrees within 10 percent (in most cases much less) with the original Hudson-Mahle result, except for  $\text{H}_2\text{O}$  and  $\text{CO}_2$ . A revised method is necessary for these two molecules, whose absorption cross sections change very rapidly over the SR band spectral range.

INTRODUCTION

The Schumann-Runge band system of molecular oxygen absorbs solar radiation in the wavelength range of 1750-2050 Å. The main transition occurs between the vibrational levels of  $B^3\Sigma_u^-$  ( $v' = 0, 1, 2, \dots$ , or 19) and of  $X^3\Sigma_g^-$  ( $v'' = 0$  or 1). This band system is the main absorber of solar UV radiation in the mesosphere, and various molecules can be photodissociated in these wavelengths in the mesosphere, lower thermosphere, and stratosphere.

Calculations of dissociation rates in Schumann-Runge band wavelengths are necessary in numerical modeling of minor constituent distributions in the upper atmosphere. Because of the very large variability of the  $\text{O}_2$  absorption cross section with wavelength and with temperature, exact calculations of radiation transmission and molecular dissociation in the Schumann-Runge bands are complicated and time consuming.

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\*Geophysical Research Laboratory, University of Tokyo, Japan

\*\*Informatics, Inc., Palo Alto, California 94303

Several methods are described in the literature for calculating the dissociation coefficients at Schumann-Runge band wavelengths by simple analytical formulae. Hudson and Mahle (refs. 1 and 2) and Kockarts (ref. 3) for example, have formulated the results of their elaborate band-to-band calculations based on their data sources into such formulae. In this report we compare the results calculated by these two methods. The main purpose of this report, however, is to present the details of a method that is simpler than previous methods in terms of economy of computer time and computer memory size necessary to store the coefficients appearing in the equations. This method was originally developed and used by Shimazaki and Ogawa (refs. 4 and 5) in their model calculations. In the present report, we demonstrate and discuss the accuracy of this method for duplicating the results obtained with the original Hudson and Mahle method.

## GENERAL EQUATIONS

The dissociation coefficient of the  $i$ th constituent, at wavelength  $\lambda$  and height  $z$ , can be calculated from the expression

$$J_i(\lambda, z) = \sigma_i(\lambda) I_\infty(\lambda) e^{-\tau(\lambda, z)} \quad (1)$$

where  $\sigma_i$  is the absorption cross section of the  $i$ th constituent,  $I_\infty$  is the intensity of the solar radiation flux at the top of the atmosphere, and  $\tau$  is the optical depth given by

$$\tau(\lambda, z) = \sum_j \sigma_j(\lambda) \int_z^\infty [X_j] dz \sec \chi \quad (2)$$

where  $[X_j]$  denotes the number density of the constituent  $X_j$ , and  $\chi$  is the solar zenith angle. The summation in equation (2) should include all constituents that contribute to absorption at wavelength  $\lambda$ , but it is sufficient in the case of the Earth's upper atmosphere to consider just  $O_2$  and  $O_3$ ; for other molecules, either  $[X_j]$  or  $\sigma_j$  are much smaller. Thus, equation (2) can be simplified as

$$\tau(\lambda, z) = \left[ \sigma_{O_2}(\lambda) \int_z^\infty [O_2] dz + \sigma_{O_3}(\lambda) \int_z^\infty [O_3] dz \right] \sec \chi \quad (3)$$

The first and the second terms on the right hand side of equation (3) will be denoted by  $\tau_{O_2}$  and  $\tau_{O_3}$ , respectively.

In order to calculate the integrated dissociation coefficient over an entire wavelength region ( $\lambda_0 - \lambda_T$ ), we divide it into a number of intervals ( $\lambda_0 - \lambda_1, \lambda_1 - \lambda_2, \dots, \lambda_{T-1} - \lambda_T$ ). This division could represent either each band or the equally divided interval in the Schumann-Runge band region. Then the total dissociation coefficient can be calculated by

$$J_i(z) = \int_{\lambda_0}^{\lambda_T} J_i(\lambda, z) d\lambda = \sum_{k=0}^{T-1} \int_{\lambda_k}^{\lambda_{k+1}} I_{\infty}(\lambda) \sigma_i(\lambda) e^{-\tau_{O_2}(\lambda, z) - \tau_{O_3}(\lambda, z)} d\lambda \quad (4)$$

Assuming that  $I_{\infty}(\lambda)$  and  $\tau_{O_3}(\lambda, z)$  are slowly varying functions of  $\lambda$ , we can write the integral in equation (4) as follows:

$$I_k = \overline{I_{\infty}(\lambda_k)} e^{-\overline{\tau_{O_3}(\lambda_k)}} \int_{\lambda_k}^{\lambda_{k+1}} \sigma_i(\lambda) e^{-\tau_{O_2}(\lambda, z)} d\lambda \quad (5)$$

where the upper bar indicates the average over the wavelength interval defined by  $\lambda_k$  and  $\lambda_{k+1}$ .

The quantity  $\sigma_{O_2}$ , and therefore  $\tau_{O_2}$ , is a strong function of  $\lambda$  in the wavelengths of Schumann-Runge band system and thus changes rapidly with  $\lambda$  over the range  $\lambda_k$  to  $\lambda_{k+1}$ . For most constituents other than  $O_2$ ,  $\sigma_i$  is generally a slowly changing function of  $\lambda$ , and the integral in equation (5) can be simplified using the averaged  $\sigma_i$  over the range of  $\lambda_k$  to  $\lambda_{k+1}$  (see later discussions for the exceptional cases of  $H_2O$  and  $CO_2$ ). Thus, we need two different kinds of integrals to calculate the dissociation rates of molecules in the Schumann-Runge region; that is

$$P(\lambda_k, z) \Delta\lambda_k = \int_{\lambda_k}^{\lambda_{k+1}} e^{-\tau_{O_2}(\lambda, z)} d\lambda \quad (6)$$

and

$$R(\lambda_k, z) \Delta\lambda_k = \int_{\lambda_k}^{\lambda_{k+1}} \sigma_{O_2}(\lambda) e^{-\tau_{O_2}(\lambda, z)} d\lambda \quad (7)$$

where  $\Delta\lambda_k = \lambda_{k+1} - \lambda_k$ .

The former integral (eq. (6)) is called the transmittance of solar radiation and can be used to calculate the total dissociation coefficient of molecules other than  $O_2$  by

$$J_M(z) = \sum_{k=0}^{T-1} \overline{I_{\infty}(\lambda_k)} \Delta\lambda_k \overline{\sigma_M(\lambda_k)} P(\lambda_k, z) e^{-\overline{\tau_{O_3}(\lambda_k)}} \quad (8)$$

and the latter integral (eq. (7)) gives the dissociation coefficient for  $O_2$  for unit solar radiation, and can be used to calculate the  $O_2$  dissociation coefficient by

$$J_{O_2}(z) = \sum_{k=0}^{T-1} \frac{\overline{I_{\infty}(\lambda_k)} \Delta \lambda_k R(\lambda_k, z) e^{-\overline{\tau_{O_2}(\lambda_k)}}}{(9)}$$

For all molecules, the total dissociation rate is calculated by multiplying the number density of the constituent and the total dissociation coefficient calculated using equations (8) or (9).

#### NUMERICAL INTEGRATION AND ANALYTICAL APPROXIMATION FORMULAE

Our purpose is to find a simple, effective, and sufficiently accurate method for calculating the integrals  $P$  and  $R$  given in equations (6) and (7). For this purpose we need to know  $\sigma_{O_2}$  as a function of  $\lambda$  and temperature. We can then evaluate  $\tau_{O_2}$  as a function of  $\sigma_{O_2}$  and  $O_2$  column density,  $N(z)$ , which appears in equation (3) as  $\int_z^{\infty} [O_2] dz \sec \chi$ .

Experimentally,  $\sigma_{O_2}$  can be evaluated only as an average over the bandwidth (resolution) of the measuring instrument. Most theoretical calculations assume a Lorentzian line shape for  $\sigma_{O_2}$  given by

$$\sigma_{O_2}(\nu) = \frac{2k_o / \pi \Delta \nu}{1 + \left[ \frac{2(\nu - \nu_i)}{\Delta \nu} \right]^2} \quad (10)$$

where  $k_o$  is the line integrated cross section,  $\nu$  is the wavenumber in  $\text{cm}^{-1}$ ,  $\nu_i$  is the wavenumber at the center of a line, and  $\Delta \nu$  is the line width. Hudson et al. (ref. 6) have determined two parameters,  $k_o$  and  $\Delta \nu$ , for each band so that the calculated  $R$  agrees with the experimental value. Based on  $k_o$  and  $\Delta \nu$ , they have calculated  $P$  and  $R$  for some chosen values of  $N$  in the range of  $10^{17}$  to  $7 \times 10^{23} \text{ cm}^{-2}$ . The effects of the underlying Schumann-Runge continuum have been incorporated in their calculations. Including the temperature dependence, they have formulated their result as

$$\ln[P(N, T)] = A + B(T - 150) + C(T - 150)^2 \quad (11)$$

and

$$\ln[R(N, T)] = D + E(T - 150) + F(T - 150)^2 \quad (12)$$

for each Schumann-Runge band, except that the bands 19-0, 18-0, and 17-0 are combined into one, and that the band 2-0 is divided into two. The wavelength divisions (19 in number) used in their (ref. 6) calculations are shown as divisions A to S in table 1. The coefficients in equations (11) and (12) are tabulated in reference 3; in each wavelength division, the coefficients A,

B, . . . , F are given for particular chosen values of  $N$ . Altogether, there are 5538 coefficients, which must be stored in computer memory in order to use this table in numerical model calculations. Furthermore, in order to calculate  $P$  and  $R$  for any value of  $N$  (or equivalently, height), the necessary coefficients must be obtained by interpolation from the coefficients available in their table. Thus, the Hudson and Mahle method needs a large computer memory for storage and also requires calculation of the necessary coefficients by interpolation.

In an attempt to simplify the numerical procedure, Shimazaki and Ogawa (refs. 4 and 5) have modified the Hudson and Mahle method. Utilizing essentially the same source of data as Hudson and Mahle (ref. 2), Shimazaki and Ogawa derived polynomial formulae of the seventh degree for computing  $P$  and  $R$  as functions of  $N$ :

$$\log P = P_0 + P_1 \log N + P_2(\log N)^2 + . . . + P_7(\log N)^7 \quad (13)$$

and

$$\log R = R_0 + R_1 \log N + R_2(\log N)^2 + . . . + R_7(\log N)^7 \quad (14)$$

Applying this method to each wavelength division of Hudson and Mahle, we have determined the coefficients  $P_i$  and  $R_i$  by the least square method. The result is shown in tables 2(a) and (b). The effect of the height-dependent temperature is incorporated in these calculations, assuming the temperature profile shown in figure 1. Since the temperature profile in this height range is not expected to change very much, the coefficients tabulated in tables 2(a) and (b) can be used without serious error in most practical cases. This method should give essentially the same result as that of Hudson and Mahle (ref. 2), but the storage requirement is reduced from 5538 to 304 and the interpolation processes can be entirely eliminated. We will refer to this method as SO(1).

In order to further reduce the computation time, Shimazaki and Ogawa (refs. 4 and 5) also changed the wavelength interval from 19 to 6, which divides the Schumann-Runge band region (1750-2050 Å) into equal intervals of 50 Å each. This division into six intervals is shown in table 3 as a part of the partition of the entire spectral range (1350-4000 Å). Above 4000 Å, the atmosphere is almost transparent, although O<sub>3</sub> (Chappuis bands) and NO<sub>2</sub> could absorb slightly at low heights (troposphere). Of 57 wavelength divisions shown in table 3, six divisions with the serial numbers 9 to 14 correspond to the Schumann-Runge band region. For each of these six divisions, the coefficients  $P_i$  and  $R_i$  have been determined for four temperatures (150, 200, 250, and 300 K) and also for the height-dependent temperatures. The results are tabulated in tables 4 through 8. We refer to this method as SO(2); it needs only 96 coefficients for storage and can reduce the computational time for the Schumann-Runge band region by a factor of about 3 over the method SO(1). We will discuss later the accuracy of the method SO(2) by comparing it with the original Hudson and Mahle method.

Table 3 includes the solar flux and absorption cross section data for the entire spectral range used in model calculations by Shimazaki and Ogawa (refs. 4 and 5) and Ogawa and Shimazaki (ref. 7). These data (except for the Schumann-Runge band region) are used in the present study to calculate the total dissociation coefficient using the Hudson model, and to compare the result with the contribution from the Schumann-Runge bands calculated according to the same model. The partition interval is generally 50 Å except for the spectral range 3100-3300 Å, where the interval 25 Å has been used. The shorter interval is preferable to this range, because the solar spectrum shows a sharp cutoff near 3100 Å and because the quantum yield for O(<sup>1</sup>D) production by O<sub>3</sub> photolyses depends upon wavelength.

Ackerman et al. (ref. 8) and Kockarts (ref. 3) calculated  $P$  and  $R$  for each band assuming a Lorentzian line shape for  $\sigma_{O_2}$  with wavenumber resolution 0.5 cm<sup>-1</sup>, which is equivalent approximately to a wavelength resolution of 0.02 Å in the Schumann-Runge band region. The values of  $\Delta\nu$ , determined by these authors on the basis of their experimental data are generally larger than those of Hudson et al. (ref. 6).

The result of elaborate calculations has been used by Kockarts (ref. 3) to construct analytical formula for calculating  $P$  and  $R$ ,

$$\ln R_b(x) = -\alpha \exp[c_1(x - x_0) + c_2(x - x_0)^2 + \dots + c_6(x - x_0)^6] \quad (15)$$

where  $R_b$  stands for either the  $P$  and  $R$  of the present paper,  $x = \ln N$ , and the values of  $x_0$ ,  $\alpha$  and  $c_i$  are tabulated in his paper for each band. The effect of temperature variation is included in the computation. The method needs 320 memory locations for storage and the computational time is about the same as that for method SO(1), but is about 3 times larger than that of method SO(2).

Kockarts (ref. 3) also determined the coefficients in equation (15) for the constant wavelength interval 10 Å and for the constant wavenumber interval 500 cm<sup>-1</sup>. The former needs 480 memory locations, and the latter requires 256 locations in order to store the coefficients. The computational time is about 5 and 3 times larger than that of method SO(2) in each case, mainly because of the increased number of divisions.

It should be noted that equation (15) cannot be used for the height range below  $x_0$ , which corresponds to about 30 km for the bands of  $v' \leq 9$  and to somewhat greater heights for the rest of the bands, because the original integral calculations of  $P$  and  $R$  were not carried out for these heights.

In table 9 we compare the computer memory size required by the various methods for storing the coefficients and the computation time relative to the method SO(2). Note that the Hudson-Mahle method needs additional time for calculating the coefficients by interpolation.



## INPUT DATA

The calculated dissociation coefficients are proportional to the incoming solar radiation flux as is seen in equations (8) and (9). The solar flux values over each wavelength division are listed in table 1 for the Schumann-Runge band region and in table 3 for the entire region of the model calculation. Most models have used the flux values compiled by Ackerman (ref. 9) and we use them for the purpose of comparison among different methods. The recent measurement by Samain and Simon (data taken from Kockarts, ref. 3) indicates much smaller fluxes in the Schumann-Runge band region, and the effect of using those data is calculated using the Kockarts method. Both sets of solar flux data are compared in figure 2.

The absorption cross section spectra of molecules which show appreciable absorption in the Schumann-Runge band region are illustrated in figure 3, and their values for the entire spectral range are listed in table 3.

The ozone density profile, which is needed to calculate  $\tau_{O_3}$  is taken from observations and is shown in figure 4. This figure also indicates the curves necessary to convert the  $O_2$  column density ( $N$ ) to the geometrical height. We have shown two curves, one for solar zenith angle  $0^\circ$  (overhead sun) and another for zenith angle  $60^\circ$  (long slant path). The  $O_2$  column density curves are based on the temperature profile shown in figure 1.

## RESULTS AND DISCUSSION

For each band, figure 5(a) compares the transmission, and figure 5(b) the  $O_2$  predissociation coefficients, of the Hudson to the Kockarts model. The Kockarts model does not provide values for the region below  $\sim 30$  km. This may not be a serious limitation for most aeronomically important stratospheric molecules, because  $H_2O$  and  $N_2O$  are decomposed mainly by chemical reaction with  $O(^1D)$  rather than by the photolysis. However, the  $N_2O$  photolysis rate could be larger than the chemical reaction rate at heights above  $\sim 22$  km.

There are significant differences between the two model results as the larger values of  $N$  are approached in each band; the Kockarts model generally gives much larger values than the Hudson model. According to Kockarts, the fine resolution used in his method for calculating the integrals  $P$  and  $R$  generally leads to a larger dissociation rate than the value calculated with the mean absorption cross sections, because the penetration of radiation through the small windows between the absorption lines is allowed. However, the very large difference between the Hudson and Kockarts results, particularly seen in the transitions from larger  $\nu'$  (shorter wavelength region), is more likely to be caused mainly by the effect of the underlying Schumann-Runge continuum, which is included in the Hudson calculation, but not in Kockarts' calculation. The underlying continuum would absorb radiation and result in a smaller transmission and  $O_2$  dissociation rate in the Hudson model than in the Kockarts model.

Near the top of the atmosphere (smaller  $N$ ) there is a slight, but systematic difference of the  $O_2$  dissociation cross sections between the Hudson and Kockarts models (see fig. 5(b)). The Hudson model tends to give a larger value than the Kockarts model for bands with  $\nu' \geq 15$ , whereas the reverse is the case for the bands with  $\nu' < 14$ . The reason for this might be a small but systematic difference of the oscillator strength measured in their experiments, although data are not available in the literature to confirm this. The dissociation coefficient at the top of the atmosphere is related to the absorption oscillator strength ( $f_{\text{abs}}$ ) by

$$\overline{J_{\infty}(\lambda)} = \frac{\pi e^2}{mc^2} f_{\text{abs}}(\lambda) \overline{I_{\infty}(\lambda)} \quad (16)$$

where  $m$  is the electron mass,  $c$  the velocity of light,  $e$  the electron charge in esu.

In figure 6 the dissociation coefficients of  $O_2$  in the Schumann-Runge bands are compared for three models labeled as Hudson, Kockarts, and Shimazaki. These three are calculated by means of equations (12), (15), and (14) with the coefficients given in Hudson and Mahle (ref. 2), Kockarts (ref. 3), and tables 4 through 8 of the present paper, respectively. In the case of the Shimazaki model, the range calculated for three temperatures (150, 250 and 300 K) is illustrated. The height scale in the abscissa corresponds to the condition of overhead sun.

The total dissociation coefficients of the Hudson model are shown by the uppermost solid curve, whereas the contributions from the Schumann-Runge bands, Schumann-Runge continuum and Herzberg continuum are shown in the lower solid curves. The comparison between the curve for the total and the curve for the Schumann-Runge bands indicates the relative importance of these bands in the height range 70-90 km, above which the Schumann-Runge continuum and below which the Herzberg continuum dominates.

The agreement among methods of the calculated dissociation coefficients in the Schumann-Runge bands is very good, as far as the same solar flux data are used. Most calculations have used the solar fluxes compiled by Ackerman (ref. 9), but the lower dashed curve is calculated for the smaller fluxes observed by Samain and Simon. Comparing this curve with the upper dashed curve calculated for the Ackerman fluxes by the same method, we find that the smaller solar fluxes give appreciably smaller dissociation coefficients; the difference is much larger than the difference caused by the choice of method.

An appreciable temperature effect is seen in Shimazaki's results, as shown in figure 6 for the height range of 80-95 km, where Schumann-Runge band absorption constitutes the major mechanism for  $O_2$  dissociation. At other heights, the temperature effect is relatively small.

The production rates of atomic oxygen from  $O_2$  and  $O_3$  photolyses are shown in figure 7, from which it is seen that the Schumann-Runge bands are the largest source between 80 and 90 km. The result is sensitive to the temperature at these heights, and use of the coefficients corresponding to a lower

temperature (table 5 for 150 K) is essential in order to reproduce, using SO(2), Hudson's result in this height range.

The calculated atomic oxygen production rate has a minimum near 90 km and a maximum near 95 km. It is interesting to note that recent rocket observations (Dickinson et al., ref. 10; Megill et al., ref. 11) indicate a minimum around 94 km and a maximum around 97 km. The height scale in our figures corresponds to an overhead sun; the scale should indicate higher levels for the oblique sun, which was the condition at the time of the rocket observations.

Figures 8(a) through 8(i) compare the dissociation coefficients of various molecules calculated by different methods. If the same solar flux is used, there is good agreement between the Hudson and Kockarts models except for  $H_2O$  and  $CO_2$ . Except for these two molecules, the absorption cross section does not change very much throughout the Schumann-Runge region (see fig. 3). Since the solar flux increases with increasing wavelengths (see fig. 2), the total dissociation comes mainly from the longer wavelength region (i.e., the transitions of smaller  $\nu'$ ). Thus, the large difference of transmission at the shorter wavelength regions (larger  $\nu'$ ) between the two models (see fig. 5(b)) does not affect the total dissociation coefficient.

The absorption cross sections of both  $H_2O$  and  $CO_2$  decrease rapidly in the Schumann-Runge band region: they decrease by six orders of magnitude for  $H_2O$  and four orders of magnitude for  $CO_2$  in the spectral range from 1950 to 2050 Å (see fig. 3). This change is much larger than the corresponding change in the solar flux, which increases about an order of magnitude for the same spectral range. Therefore, the contribution from the shorter wavelength region (or the transitions of larger  $\nu'$ ) to the total dissociation rate in the Schumann-Runge band region becomes larger. It is in these transitions that the Kockarts model calculates an appreciably larger transmission than the Hudson model (see fig. 5(a)). Thus, the total dissociation rates for  $H_2O$  and  $CO_2$  are generally larger in the Kockarts model than in the Hudson model. The magnitude of this difference could be comparable to the difference caused by use of the two different solar spectra for the height region of  $N > 10^{21} \text{ cm}^{-2}$  in the case of  $H_2O$ , and of  $10^{22} > N > 10^{20} \text{ cm}^{-2}$  in case of  $CO_2$ . At other heights for  $H_2O$  and  $CO_2$ , and also over the entire height range for other molecules, the effect of changing the solar spectrum is much larger than the effect of using different methods.

Of nine molecules shown in figures 8(a) through 8(i),  $H_2O$  dissociation occurs almost exclusively in the Schumann-Runge band region, as does a small fraction (<5 percent) of  $H_2O_2$  dissociation (note the reduction by a factor of 10 for illustrating a total rate curve in fig. 8(f)). For most other molecules, dissociation in Schumann-Runge band system is comparable to dissociation at other parts of the spectral range. As is seen in table 3,  $HNO_3$  and  $H_2O_2$  have appreciable absorption at wavelengths longer than the Schumann-Runge bands, and the contribution from this spectral range becomes dominant as we go to lower heights.

The method SO(2) was derived to reproduce the Hudson model result, but with much less computer time and memory core for storage. In figures 6 and 8,

the results calculated by the method SO(2) are shown by short vertical lines for the range  $T = 150$  to  $300$  K. A cross on the line indicates the result for  $T = 250$  K. The result generally agrees well with the Hudson model result. As is seen in table 10, the difference is generally within 10 percent (in most cases a much smaller percentage) except for  $H_2O$  and  $CO_2$ , if the coefficients for appropriate temperatures are used. The temperature effect is particularly large in the lower stratosphere (larger  $N$ ); a larger temperature gives a smaller value, whereas a smaller temperature gives a larger value, for the dissociation coefficient. The difference between two cases of  $150$  K and  $300$  K in the lower stratosphere can be as large as 40 percent, whereas the difference in the upper regions is much smaller. The results calculated for the height-dependent temperature using the coefficients in table 8 give the smallest difference for the entire height (or  $N$  value) range, although the difference is sometimes larger than the result of constant temperature for some particular value of  $N$ . For  $H_2O$  and  $CO_2$  the absorption cross sections vary greatly over the  $50 \text{ \AA}$  interval, and the use of the mean cross section in equation (8) would certainly cause a large error.

## CONCLUSIONS

The major conclusions that may be drawn from this study are summarized as follows:

1. Except for  $H_2O$  and  $CO_2$ , calculations by the Hudson-Mahle method and Kockarts method are in good agreement over the whole Schumann-Runge bands, provided that the same solar flux data are used. However, occasionally calculations for each band reveal significant differences between the two models, particularly in the shorter wavelength region (transitions of larger  $\nu'$ ), due mainly to effects of the underlying Schumann-Runge continuum that were included in the Hudson model but not in the Kockarts model.
2. Effects of using different solar flux data are generally much larger than effects caused by different methods of calculation. In a model using equally divided intervals, it is essential to sum the solar fluxes at each band within that interval rather than to use the mean solar flux multiplied by the wavelength interval.
3. The temperature effect on the  $O_2$  dissociation coefficients is most pronounced in the mesosphere, whereas the effect is strongest in the stratosphere for other molecules.
4. Method SO(2) provides the most economical method in calculating the photodissociation rates in the Schumann-Runge band region. Except for  $H_2O$  and  $CO_2$ , calculation by this method yields results which agree within 10 percent (usually much less) with the result of the original Hudson and Mahle method as long as temperature effects are properly taken into account.
5. The absorption cross sections of  $H_2O$  and  $CO_2$  change greatly over the Schumann-Runge band region ( $1750$ - $2050 \text{ \AA}$ ) and even over the  $50 \text{ \AA}$  interval.

within this region. This causes a large difference between the result calculated by  $SO(2)$  and that by the Hudson method. An improved method has to be developed for these two constituents.

Ames Research Center  
National Aeronautics and Space Administration  
Moffett Field, California 94035, Nov. 8, 1976

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TABLE 1.- SCHUMANN-RUNGE BANDS ( $\nu'$  - 0) AND SOLAR FLUXES; THE DIVISION A, B, . . . , S  
CORRESPONDS TO THE DIVISIONS IN HUDSON AND MAHLE, (REF. 2)

Division	Band	Wavelength range, Å	$\Delta\lambda$	Solar flux, cm <sup>-2</sup> sec <sup>-1</sup>	
				Ackerman (ref. 9)	Samain and Simon
A	19-0	1753.40 - 1755.79	2.39	2.99(10)*	1.50(10)
A	18-0	1755.79 - 1758.94	3.15	4.41(10)	2.10(10)
A	17-0	1758.94 - 1763.20	4.26	6.30(10)	2.81(10)
B	16-0	1763.20 - 1768.60	5.40	8.10(10)	3.84(10)
C	15-0	1768.60 - 1774.60	6.00	9.30(10)	6.40(10)
D	14-0	1774.60 - 1782.60	8.00	1.32(11)	8.38(10)
E	13-0	1782.60 - 1792.60	10.00	1.74(11)	1.26(11)
F	12-0	1792.60 - 1803.60	11.00	2.01(11)	1.56(11)
G	11-0	1803.60 - 1816.40	12.80	2.51(11)	2.08(11)
H	10-0	1816.40 - 1830.60	14.20	3.14(11)	2.91(11)
I	9-0	1830.60 - 1846.20	15.60	3.90(11)	3.13(11)
J	8-0	1846.20 - 1863.40	17.20	4.83(11)	3.42(11)
K	7-0	1863.40 - 1882.20	18.80	5.99(11)	4.98(11)
L	6-0	1882.20 - 1902.40	20.20	7.22(11)	6.02(11)
M	5-0	1902.40 - 1924.00	21.60	8.73(11)	7.58(11)
N	4-0	1924.00 - 1947.00	23.00	1.27(12)	8.15(11)
O	3-0	1947.00 - 1971.80	24.80	1.73(12)	1.22(12)
P	2-0	1971.80 - 1985.00	13.20	9.82(11)	1.38(12)
Q	2-0	1985.00 - 2000.00	15.00	1.15(12)	1.38(12)
R	1-0	2000.00 - 2025.00	25.00	2.01(12)	1.79(12)
S	0-0	2025.00 - 2050.00	25.00	2.32(12)	1.09(12)

\*Numeral A(k) should read as  $A \times 10^k$ .

TABLE 2.- COEFFICIENTS TO CALCULATE THE TRANSMITTANCE AND THE O<sub>2</sub> DISSOCIATION RATES IN METHOD SO(1) FOR THE HEIGHT-DEPENDENT TEMPERATURE

(a) Coefficients in equation (13)								
Division	P <sub>0</sub>	P <sub>1</sub>	P <sub>2</sub>	P <sub>3</sub>	P <sub>4</sub>	P <sub>5</sub>	P <sub>6</sub>	P <sub>7</sub>
A	9.64245(5)*	-3.86520(5)	6.63259(4)	-6.31624(3)	3.60544(2)	-1.23373(1)	2.34350(-1)	-1.90650(-3)
B	3.60957(5)	-1.47330(5)	2.57512(4)	-2.49860(3)	1.45356(2)	-5.07029(0)	9.81961(-2)	-8.14599(-4)
C	6.25465(5)	-2.50109(5)	4.28066(4)	-4.06510(3)	2.31343(2)	-7.89027(0)	1.49341(-1)	-1.21015(-3)
D	1.93183(5)	-7.73955(4)	1.32748(4)	-1.26368(3)	7.21101(1)	-2.46683(0)	4.68463(-2)	-3.81011(-4)
E	2.99191(5)	-1.18707(5)	2.01547(4)	-1.89835(3)	1.07134(2)	-3.62283(0)	6.79744(-2)	-5.45934(-4)
F	3.40140(5)	-1.33875(5)	2.25420(4)	-2.10506(3)	1.17750(1)	-3.94555(0)	7.33340(-2)	-5.83283(-4)
G	-1.15218(4)	2.96190(3)	-2.25539(2)	-5.22146(0)	1.80514(0)	-1.12618(-1)	3.08878(-3)	-3.27011(-5)
H	4.88031(4)	-1.94837(4)	3.32989(3)	-3.15830(2)	1.79550(1)	-6.11863(-1)	1.15734(-2)	-9.37435(-5)
I	1.13279(5)	-4.37784(4)	7.23463(3)	-6.62764(2)	3.63540(1)	-1.19410(0)	2.17497(-2)	-1.69489(-4)
J	1.15250(5)	-4.41354(4)	7.22532(3)	-6.55542(2)	3.56034(1)	-1.15768(0)	2.08702(-2)	-1.60947(-4)
K	2.00108(5)	-7.63581(4)	1.24593(4)	-1.12578(3)	6.08593(1)	-1.96856(0)	3.52798(-2)	-2.70266(-4)
L	1.71838(5)	-6.50794(4)	1.05284(4)	-9.43188(2)	5.05355(1)	-1.61951(0)	2.87452(-2)	-2.18007(-4)
M	1.52518(5)	-5.77643(4)	9.34530(3)	-8.37233(2)	4.48605(1)	-1.43771(0)	2.55198(-2)	-1.93557(-4)
N	1.65441(5)	-6.24491(4)	1.00680(4)	-8.98693(2)	4.79711(1)	-1.53133(0)	2.70698(-2)	-2.04434(-4)
O	1.17195(5)	-4.42395(4)	7.13295(3)	-6.36809(2)	3.39998(1)	-1.08567(0)	1.91990(-2)	-1.45060(-4)
P	1.10275(5)	-4.16687(4)	6.72545(3)	-6.01086(2)	3.21294(1)	-1.02718(0)	1.81873(-2)	-1.37594(-4)
Q	1.64614(5)	-6.19277(4)	9.94959(3)	-8.85013(2)	4.70722(1)	-1.49718(0)	2.63681(-2)	-1.98383(-4)
R	1.59108(5)	-5.98622(4)	9.61871(3)	-8.55674(2)	4.55169(1)	-1.44788(0)	2.55030(-2)	-1.91900(-4)
S	1.50431(5)	-5.65992(4)	9.09466(3)	-8.09080(2)	4.30399(1)	-1.36914(0)	2.41172(-2)	-1.81480(-4)

(b) Coefficients in equation (14)								
Division	R <sub>0</sub>	R <sub>1</sub>	R <sub>2</sub>	R <sub>3</sub>	R <sub>4</sub>	R <sub>5</sub>	R <sub>6</sub>	R <sub>7</sub>
A	-2.23178(5)*	8.56837(4)	-1.40281(4)	1.26875(3)	-6.84122(1)	2.19706(0)	-3.88602(-2)	2.91491(-4)
B	-5.37174(5)	2.05232(5)	-3.34300(4)	3.00810(3)	-1.61403(2)	5.16081(0)	-9.09771(-2)	6.81390(-4)
C	5.05218(4)	-2.38634(4)	4.74207(3)	-5.15770(2)	3.32375(1)	-1.27127(0)	2.67574(-2)	-2.39337(-4)
D	2.86001(5)	-1.10136(5)	1.81685(4)	-1.66501(3)	9.15777(1)	-3.02391(0)	5.55211(-2)	-4.37388(-4)
E	3.09553(5)	-1.20294(5)	2.00281(4)	-1.85244(3)	1.02816(2)	-3.42490(0)	6.34065(-2)	-5.03326(-4)
F	7.97225(4)	-3.36020(4)	6.05275(3)	-6.04004(2)	3.60534(1)	-1.28701(0)	2.54360(-2)	-2.14680(-4)
G	-1.79013(5)	6.55222(4)	-1.01929(4)	8.72743(2)	-4.43694(1)	1.33735(0)	-2.20843(-2)	1.53700(-4)
H	-1.05587(5)	3.98373(4)	-6.39757(3)	5.66511(2)	-2.98583(1)	9.36092(-1)	-1.61519(-2)	1.18214(-4)
I	-7.39158(4)	2.69609(4)	-4.17706(3)	3.55897(2)	-1.79889(1)	5.38582(-1)	-8.82599(-3)	6.08976(-5)
J	-5.69086(4)	2.01018(4)	-3.00458(3)	2.45731(2)	-1.18416(1)	3.34809(-1)	-5.10954(-3)	3.21228(-5)
K	1.25324(5)	-4.88466(4)	8.13325(3)	-7.50024(2)	-1.36466(1)	-1.36466(0)	2.49293(-2)	-1.94543(-4)
L	1.06603(5)	-4.11253(4)	6.77582(3)	-6.18144(2)	3.37201(1)	-1.09986(0)	1.98607(-2)	-1.53161(-4)
M	1.46641(5)	-5.60523(4)	9.14826(3)	-8.26508(2)	4.46411(1)	-1.44144(0)	2.57640(-2)	-1.96648(-4)
N	2.45343(5)	-9.24469(4)	1.48704(4)	-1.32377(3)	7.04348(1)	-2.24007(0)	3.94300(-2)	-2.96348(-4)
O	1.78028(5)	-6.68633(4)	1.07193(4)	-9.51038(2)	5.04335(1)	-1.59866(0)	2.80486(-2)	-2.10146(-4)
P	1.61656(5)	-6.09003(4)	9.79459(3)	-8.71895(2)	4.63969(1)	-1.47597(0)	2.59912(-2)	-1.95462(-4)
Q	1.84740(5)	-6.93295(4)	1.11064(4)	-9.84724(2)	5.21919(1)	-1.65379(0)	2.90116(-2)	-2.17379(-4)
R	1.60886(5)	-6.05304(4)	9.72364(3)	-8.64714(2)	4.59784(1)	-1.46185(0)	2.57351(-2)	-1.93532(-4)
S	1.52009(5)	-5.71919(4)	9.18791(3)	-8.17159(2)	4.34562(1)	-1.38191(0)	2.43329(-2)	-1.83031(-4)

\*Numerical A(k) should read as  $A \times 10^k$ .



TABLE 3.- THE INTEGRATED SOLAR FLUX AND THE MEAN ABSORPTION CROSS SECTIONS FOR VARIOUS MOLECULES OVER EACH OF 57 WAVELENGTH DIVISIONS  
IN THE SPECTRUM RANGE OF 1350-4000 Å

Division	Wavelength, Å	Solar flux, cm <sup>-2</sup> sec <sup>-1</sup>	Mean absorption cross sections, cm <sup>-2</sup>										
			O <sub>2</sub>	O <sub>3</sub>	N <sub>2</sub> O	H <sub>2</sub> O	H <sub>2</sub> O <sub>2</sub>	HNO <sub>3</sub>	HCl	SO <sub>2</sub>	CFCl <sub>3</sub>	CF <sub>2</sub> Cl <sub>2</sub>	CO <sub>2</sub>
1	1350-1400	1.40(10)*	6.70(-18)	1.60(-17)	4.80(-18)	3.40(-18)	7.80(-18)	0	7.60(-19)	0	3.40(-17)	1.20(-18)	7.00(-19)
2	1400-1450	1.93(10)	1.38(-17)	7.70(-18)	1.08(-18)	8.40(-19)	5.60(-18)	0	1.40(-18)	3.16(-18)	1.30(-17)	3.80(-19)	5.20(-19)
3	1450-1500	3.50(10)	1.43(-17)	5.10(-18)	6.60(-18)	5.10(-19)	4.10(-18)	0	2.20(-18)	4.22(-18)	5.20(-18)	1.90(-19)	6.30(-19)
4	1500-1550	5.50(10)	1.12(-17)	3.90(-18)	1.90(-18)	1.07(-18)	3.60(-18)	0	3.00(-18)	5.62(-18)	3.60(-18)	2.10(-19)	5.20(-19)
5	1550-1600	8.25(10)	7.90(-18)	2.00(-18)	1.02(-19)	2.30(-18)	3.30(-18)	0	3.30(-18)	3.65(-18)	3.50(-18)	2.90(-19)	3.70(-19)
6	1600-1650	1.20(11)	4.80(-18)	1.15(-18)	3.70(-20)	3.60(-18)	3.70(-18)	0	2.70(-18)	1.33(-18)	5.20(-18)	1.80(-19)	1.70(-19)
7	1650-1700	1.98(11)	2.20(-18)	8.30(-19)	5.80(-20)	4.60(-18)	3.90(-18)	7.10(-18)	2.00(-18)	4.22(-19)	6.20(-18)	2.00(-19)	7.20(-20)
8	1700-1750	3.60(11)	6.70(-19)	8.10(-19)	9.30(-20)	3.60(-18)	3.20(-18)	9.40(-18)	1.20(-18)	4.87(-19)	5.20(-18)	3.20(-19)	1.30(-20)
9	1750-1800	8.17(11)	1.30(-23)	8.30(-19)	1.34(-19)	1.85(-18)	1.71(-18)	1.29(-17)	6.20(-19)	1.00(-18)	5.00(-18)	4.60(-19)	2.90(-21)
10	1800-1850	1.12(12)	1.31(-23)	6.90(-19)	1.41(-19)	2.20(-19)	1.18(-18)	1.30(-17)	3.60(-19)	1.78(-18)	5.20(-18)	5.40(-19)	5.80(-22)
11	1850-1900	1.61(12)	1.33(-23)	6.00(-19)	1.26(-19)	1.50(-20)	1.05(-18)	1.15(-17)	1.70(-19)	4.22(-18)	2.40(-18)	9.00(-19)	1.35(-22)
12	1900-1950	2.43(12)	1.31(-23)	4.50(-19)	9.70(-20)	1.60(-21)	6.70(-19)	1.13(-17)	9.00(-20)	4.22(-18)	1.90(-18)	6.00(-19)	2.70(-23)
13	1950-2000	3.64(12)	1.25(-23)	3.60(-19)	6.00(-20)	1.75(-22)	5.60(-19)	7.20(-18)	3.60(-20)	3.16(-18)	1.10(-18)	2.40(-19)	8.00(-24)
14	2000-2050	4.33(12)	1.20(-23)	3.05(-19)	2.80(-20)	1.50(-23)	4.90(-19)	3.70(-18)	1.60(-20)	2.37(-18)	6.50(-19)	8.60(-20)	3.70(-24)
15	2050-2100	7.50(12)	1.18(-23)	3.75(-19)	1.48(-20)		4.40(-19)	2.10(-18)	7.20(-21)	1.78(-18)	3.50(-19)	3.10(-20)	3.10(-24)
16	2100-2150	1.63(13)	1.08(-23)	5.30(-19)	7.10(-21)		4.00(-19)	9.70(-19)	3.70(-21)	1.15(-18)	1.60(-19)	1.20(-20)	2.80(-24)
17	2150-2200	2.50(13)	9.30(-24)	9.50(-19)	2.90(-21)		3.40(-19)	3.28(-19)	1.50(-21)	5.62(-19)	6.20(-20)	2.10(-21)	2.20(-24)
18	2200-2250	3.45(13)	7.30(-24)	1.80(-18)	1.15(-21)		2.80(-19)	1.44(-19)		2.37(-19)	2.20(-20)	4.00(-22)	
19	2250-2300	4.15(13)	5.00(-24)	2.90(-18)	4.80(-22)		2.40(-19)	8.51(-21)		1.33(-19)	1.00(-20)		
20	2300-2350	4.40(13)	2.90(-24)	4.40(-18)	5.00(-23)		2.05(-19)	5.63(-20)		2.05(-20)	3.80(-21)		
21	2350-2400	4.00(13)	1.40(-24)	6.20(-18)	2.00(-23)		1.70(-19)	3.74(-20)			1.30(-21)		
22	2400-2450	3.90(13)	3.10(-25)	8.10(-18)	5.00(-24)		1.40(-19)	2.60(-20)					
23	2450-2500	4.25(13)		9.80(-18)	2.00(-24)		1.15(-19)	2.10(-20)					
24	2500-2550	4.75(13)		1.10(-17)	6.00(-25)		1.02(-19)	1.95(-20)					
25	2550-2600	6.00(13)		1.10(-17)	4.00(-25)		8.30(-20)	1.94(-20)					
26	2600-2650	1.00(14)		1.07(-17)	2.50(-25)		6.90(-20)	1.90(-20)					
27	2650-2700	1.50(14)		9.80(-18)	1.00(-25)		5.40(-20)	1.80(-20)					
28	2700-2750	1.85(14)		7.70(-18)			4.10(-20)	1.63(-20)					
29	2750-2800	1.80(14)		5.80(-18)			3.10(-20)	1.40(-20)					
30	2800-2850	1.88(14)		3.80(-18)			2.40(-20)	1.14(-20)					
31	2850-2900	2.50(14)		2.40(-18)			1.90(-20)	8.77(-21)					
32	2900-2950	3.75(14)		1.43(-18)			1.50(-20)	6.34(-21)					
33	2950-3000	4.50(14)		7.50(-19)			1.20(-20)	4.26(-21)					
34	3000-3050	4.50(14)		3.75(-19)			1.00(-20)	2.76(-21)					
35	3050-3100	5.00(14)		1.93(-19)			8.00(-21)	1.68(-21)					
36	3100-3125	2.75(14)		1.28(-19)			7.00(-21)	9.50(-22)					
37	3125-3150	3.13(14)		9.00(-20)			6.45(-21)	7.10(-22)					
38	3150-3175	3.38(14)		6.33(-20)			5.90(-21)	4.70(-22)					
39	3175-3200	3.63(14)		4.75(-20)			5.45(-21)	3.25(-22)					
40	3200-3225	3.88(14)		3.50(-20)			5.00(-21)	1.80(-22)					
41	3225-3250	4.00(14)		2.25(-20)			4.75(-21)	1.00(-22)					
42	3250-3275	4.25(14)		1.80(-20)			4.50(-21)	2.00(-23)					
43	3275-3300	4.38(14)		1.00(-20)			4.25(-21)	1.00(-23)					
44	3300-3350	9.00(14)		6.40(-21)			4.00(-21)						
45	3350-3400	9.25(14)		3.20(-21)			3.50(-21)						
46	3400-3450	9.75(14)		1.47(-21)			3.00(-21)						
47	3450-3500	1.00(15)		6.70(-22)			2.60(-21)						
48	3500-3550	1.03(15)		3.00(-22)			2.20(-21)						
49	3550-3600	1.05(15)		1.30(-22)			1.90(-21)						
50	3600-3650	1.05(15)		4.00(-23)			1.50(-21)						
51	3650-3700	1.18(15)		0.			1.20(-21)						
52	3700-3750	1.23(15)		0.			8.70(-22)						
53	3750-3800	1.23(15)		0.									
54	3800-3850	1.15(15)		0.									
55	3850-3900	1.10(15)		0.									
56	3900-3950	1.10(15)		0.									
57	3950-4000	1.18(15)		0.									

\*Numeral A(k) should read as A×10<sup>k</sup>

TABLE 4.- COEFFICIENTS TO CALCULATE THE TRANSMITTANCE AND THE O<sub>2</sub> DISSOCIATION RATES IN METHOD SO(2) FOR THE TEMPERATURE 150 K

(a) Coefficients in equation (13)								
Division	P <sub>0</sub>	P <sub>1</sub>	P <sub>2</sub>	P <sub>3</sub>	P <sub>4</sub>	P <sub>5</sub>	P <sub>6</sub>	P <sub>7</sub>
9	1.08163(5)*	-4.36764(4)	7.54442(3)	-7.22630(2)	4.14515(1)	-1.42398(0)	2.71263(-2)	-2.21064(-4)
10	9.90159(4)	-3.86648(4)	6.45620(3)	-5.97597(2)	3.31170(1)	-1.09882(0)	2.02134(-2)	-1.59044(-4)
11	4.14770(4)	-1.59751(4)	2.63012(3)	-2.39958(2)	1.31033(1)	-4.28297(-1)	7.75988(-3)	-6.01254(-5)
12	1.12919(5)	-4.29609(4)	6.98196(3)	-6.28339(2)	3.38191(1)	-1.08868(0)	1.94090(-2)	-1.47841(-4)
13	1.02245(5)	-3.88122(4)	6.29303(3)	-5.64979(2)	3.03337(1)	-9.73997(-1)	1.73191(-2)	-1.31567(-4)
14	1.08779(5)	-4.12757(4)	6.68954(3)	-6.00299(2)	3.22141(1)	-1.03382(0)	1.83724(-2)	-1.39483(-4)

(b) Coefficients in equation (14)								
Division	R <sub>0</sub>	R <sub>1</sub>	R <sub>2</sub>	R <sub>3</sub>	R <sub>4</sub>	R <sub>5</sub>	R <sub>6</sub>	R <sub>7</sub>
9	1.49188(5)	-6.10004(4)	1.06590(4)	-1.03181(3)	5.97557(1)	-2.07022(0)	3.97252(-2)	-3.25693(-4)
10	7.59127(3)	-4.04242(3)	8.62047(2)	-9.77888(1)	6.44842(0)	-2.48941(-1)	5.23358(-3)	-4.63733(-5)
11	-1.76776(3)	-3.99100(2)	2.43967(2)	-3.85736(1)	2.99367(0)	-1.26513(-1)	2.80113(-3)	-2.55381(-5)
12	1.54261(5)	-5.90490(4)	9.64901(3)	-8.72585(2)	4.71617(1)	-1.52339(0)	2.72295(-2)	-2.07764(-4)
13	2.01203(5)	-7.60616(4)	1.22747(4)	-1.09628(3)	5.85215(1)	-1.86726(0)	3.29741(-2)	-2.48619(-4)
14	1.20114(5)	-4.55305(4)	7.36960(3)	-6.60406(2)	3.53867(1)	-1.13383(0)	2.01152(-2)	-1.52437(-4)

\*Numeral A(k) should read as  $A \times 10^k$ .TABLE 5.- COEFFICIENTS TO CALCULATE THE TRANSMITTANCE AND THE O<sub>2</sub> DISSOCIATION RATES IN METHOD SO(2) FOR THE TEMPERATURE 200 K

(a) Coefficients in equation (13)								
Division	P <sub>0</sub>	P <sub>1</sub>	P <sub>2</sub>	P <sub>3</sub>	P <sub>4</sub>	P <sub>5</sub>	P <sub>6</sub>	P <sub>7</sub>
9	1.96036(5)*	-7.80681(4)	1.33010(4)	-1.25683(3)	7.11343(1)	-2.41158(0)	4.53451(-2)	-3.64821(-4)
10	1.08986(5)	-4.23452(4)	7.03569(3)	-6.48041(2)	3.57390(1)	-1.18020(0)	2.16101(-2)	-1.69270(-4)
11	1.16123(5)	-4.40549(4)	7.14072(3)	-6.41050(2)	3.44268(1)	-1.10609(0)	1.96874(-2)	-1.49773(-4)
12	1.36331(5)	-5.16006(4)	8.34279(3)	-7.46943(2)	3.99972(1)	-1.28104(0)	2.27241(-2)	-1.72240(-4)
13	1.98379(5)	-7.45194(4)	1.19541(4)	-1.06161(3)	5.63704(1)	-1.78980(0)	3.14651(-2)	-2.36292(-4)
14	1.53176(5)	-5.76353(4)	9.26175(3)	-8.24002(2)	4.38367(1)	-1.39459(0)	2.45673(-2)	-1.84881(-4)

(b) Coefficients in equation (14)								
Division	R <sub>0</sub>	R <sub>1</sub>	R <sub>2</sub>	R <sub>3</sub>	R <sub>4</sub>	R <sub>5</sub>	R <sub>6</sub>	R <sub>7</sub>
9	2.12571(5)	-8.57646(4)	1.47986(4)	-1.41561(3)	8.10690(1)	-2.77918(0)	5.28044(-2)	-4.28929(-4)
10	-1.55042(4)	4.83256(3)	-5.95733(2)	3.49003(1)	-7.80037(-1)	-1.32515(-2)	9.74658(-4)	-1.34721(-5)
11	8.03231(3)	-4.11842(3)	8.45482(2)	-9.23056(1)	5.85665(0)	-2.17503(-1)	4.39831(-3)	-3.74845(-5)
12	1.87325(5)	-7.11816(4)	1.15484(4)	-1.03706(3)	5.56698(1)	-1.78636(0)	3.17269(-2)	-2.40602(-4)
13	2.51679(5)	-9.44945(4)	1.51462(4)	-1.34366(3)	7.12527(1)	-2.25866(0)	3.96309(-2)	-2.96941(-4)
14	1.52335(5)	-5.73294(4)	9.21296(3)	-8.19702(2)	4.36107(1)	-1.38750(0)	2.44446(-2)	-1.83976(-4)

\*Numeral A(k) should read as  $A \times 10^k$ .

TABLE 6.- COEFFICIENTS TO CALCULATE THE TRANSMITTANCE AND THE O<sub>2</sub> DISSOCIATION RATES IN METHOD SO(2) FOR THE TEMPERATURE 250 K

(a) Coefficients in equation (13)								
Division	P <sub>0</sub>	P <sub>1</sub>	P <sub>2</sub>	P <sub>3</sub>	P <sub>4</sub>	P <sub>5</sub>	P <sub>6</sub>	P <sub>7</sub>
9	1.73786(5)*	-6.95971(4)	1.19236(4)	-1.13285(3)	6.44629(1)	-2.19698(0)	4.15251(-2)	-3.35795(-4)
10	1.24912(5)	-4.85446(4)	8.06623(3)	-7.42874(2)	4.09564(1)	-1.35182(0)	2.47353(-2)	-1.93577(-4)
11	6.50601(4)	-2.48561(4)	4.05765(3)	-3.66920(2)	1.98509(1)	-6.42600(-1)	1.15260(-2)	-8.83798(-5)
12	1.08752(5)	-4.13879(4)	6.72861(3)	-6.05778(2)	3.26197(1)	-1.05062(0)	1.87422(-2)	-1.42865(-4)
13	1.01484(5)	-3.85372(4)	6.25082(3)	-5.61420(2)	3.01559(1)	-9.68744(-1)	1.72344(-2)	-1.30995(-4)
14	1.08702(5)	-4.12487(4)	6.68555(3)	-5.99977(2)	3.21990(1)	-1.03341(0)	1.83665(-2)	-1.39450(-4)
(b) Coefficients in equation (14)								
Division	R <sub>0</sub>	R <sub>1</sub>	R <sub>2</sub>	R <sub>3</sub>	R <sub>4</sub>	R <sub>5</sub>	R <sub>6</sub>	R <sub>7</sub>
9	2.03153(5)	-8.26752(4)	1.43801(4)	-1.38579(3)	7.99048(1)	-2.75653(0)	5.26774(-2)	-4.30174(-4)
10	1.27615(4)	-6.08681(3)	1.20471(3)	-1.29348(2)	8.17326(0)	-3.04885(-1)	6.23080(-3)	-5.39116(-5)
11	-3.07120(4)	1.07858(4)	-1.60420(3)	1.30689(2)	-6.28491(0)	1.77891(-1)	-2.73213(-3)	1.74449(-5)
12	1.50342(5)	-5.72943(4)	9.32189(3)	-8.39481(2)	4.51905(1)	-1.45415(0)	2.58985(-2)	-1.96949(-4)
13	1.36436(5)	-5.15881(4)	8.32721(3)	-7.43976(2)	3.97337(1)	-1.26857(0)	2.24189(-2)	-1.69194(-4)
14	9.39704(4)	-3.57067(4)	5.79409(3)	-5.20618(2)	2.79762(1)	-8.99109(-1)	1.60024(-2)	-1.21680(-4)

\*Numeral A(k) should read as A×10<sup>k</sup>.TABLE 7.- COEFFICIENTS TO CALCULATE THE TRANSMITTANCE AND THE O<sub>2</sub> DISSOCIATION RATES IN METHOD SO(2) FOR THE TEMPERATURE 300 K

(a) Coefficients in equation (13)								
Division	P <sub>0</sub>	P <sub>1</sub>	P <sub>2</sub>	P <sub>3</sub>	P <sub>4</sub>	P <sub>5</sub>	P <sub>6</sub>	P <sub>7</sub>
9	1.65842(5)*	-6.67551(4)	1.14943(4)	-1.09747(3)	6.27528(1)	-2.14886(0)	4.08038(-2)	-3.31453(-4)
10	1.48480(5)	-5.75904(4)	9.54942(3)	-8.77549(2)	4.82703(1)	-1.58939(0)	2.90091(-2)	-2.26428(-4)
11	8.22737(4)	-3.13677(4)	5.10929(3)	-4.60917(2)	2.48726(1)	-8.02964(-1)	1.43604(-2)	-1.09772(-4)
12	1.13444(5)	-4.31547(4)	7.01286(3)	-6.31112(2)	3.39709(1)	-1.09376(0)	1.95058(-2)	-1.48650(-4)
13	1.01843(5)	-3.86748(4)	6.27350(3)	-5.63500(2)	3.02707(1)	-9.72559(-1)	1.73051(-2)	-1.31559(-4)
14	1.08377(5)	-4.11295(4)	6.66699(3)	-5.98385(2)	3.21177(1)	-1.03095(0)	1.83255(-2)	-1.39160(-4)
(b) Coefficients in equation (14)								
Division	R <sub>0</sub>	R <sub>1</sub>	R <sub>2</sub>	R <sub>3</sub>	R <sub>4</sub>	R <sub>5</sub>	R <sub>6</sub>	R <sub>7</sub>
9	2.62274(5)	-1.05989(5)	1.83105(4)	-1.75301(3)	1.00440(2)	-3.44388(0)	6.54280(-2)	-5.31302(-4)
10	7.12464(4)	-2.85659(4)	4.89537(3)	-4.64869(2)	2.64146(1)	-8.97983(-1)	1.69096(-2)	-1.36054(-4)
11	8.04692(4)	-3.12290(4)	5.17513(3)	-4.74786(2)	2.60421(1)	-8.53945(-1)	1.54996(-2)	-1.20130(-4)
12	1.31662(5)	-5.02897(4)	8.20078(3)	-7.40207(2)	3.99385(1)	-1.28816(0)	2.29975(-2)	-1.75322(-4)
13	1.83427(5)	-6.93047(4)	1.11789(4)	-9.97990(2)	5.32574(1)	-1.69891(0)	2.99980(-2)	-2.26186(-4)
14	1.20645(5)	-4.57333(4)	7.40270(3)	-6.63405(2)	3.55496(1)	-1.13913(0)	2.02111(-2)	-1.53180(-4)

\*Numeral A(k) should read as A×10<sup>k</sup>.

TABLE 8.- COEFFICIENTS TO CALCULATE THE TRANSMITTANCE AND THE O<sub>2</sub> DISSOCIATION RATES IN METHOD SO(2)  
FOR THE HEIGHT-DEPENDENT TEMPERATURE

(a) Coefficients in equation (13)								
Division	P <sub>0</sub>	P <sub>1</sub>	P <sub>2</sub>	P <sub>3</sub>	P <sub>4</sub>	P <sub>5</sub>	P <sub>6</sub>	P <sub>7</sub>
9	2.425470(5)*	-9.624982(4)	1.634189(4)	-1.538926(3)	8.681247(1)	-2.933657(0)	5.499110(-2)	-4.411116(-4)
10	9.669204(4)	-3.720173(4)	6.120147(3)	-5.581338(2)	3.047686(1)	-9.965949(-1)	1.807304(-2)	-1.402446(-4)
11	1.758494(5)	-6.642738(4)	1.071749(4)	-9.574185(2)	5.114708(1)	-1.634098(0)	2.891237(-2)	-2.185616(-4)
12	1.594939(5)	-6.022813(4)	9.714026(3)	-8.674938(2)	4.632826(1)	-1.479664(0)	2.617115(-2)	-1.977668(-4)
13	1.999395(5)	-7.509682(4)	1.204521(4)	-1.069549(3)	5.678393(1)	-1.802658(0)	3.168603(-2)	-2.379107(-4)
14	1.536738(5)	-5.782068(4)	9.291203(3)	-8.265891(2)	4.397255(1)	-1.398852(0)	2.464124(-2)	-1.854291(-4)
(b) Coefficients in equation (14)								
Division	R <sub>0</sub>	R <sub>1</sub>	R <sub>2</sub>	R <sub>3</sub>	R <sub>4</sub>	R <sub>5</sub>	R <sub>6</sub>	R <sub>7</sub>
9	2.513007(5)	-1.009141(5)	1.733542(4)	-1.651368(3)	9.420378(1)	-3.217900(0)	6.093978(-2)	-4.935429(-4)
10	-9.579851(4)	3.591625(4)	-5.737624(3)	5.060408(2)	-2.660443(1)	8.334936(-1)	-1.440281(-2)	1.058476(-4)
11	6.218042(4)	-2.412592(4)	3.998560(3)	-3.670430(2)	2.015139(1)	-6.616500(-1)	1.202909(-2)	-9.341187(-5)
12	1.845680(5)	-6.993932(4)	1.131505(4)	-1.013242(3)	5.423934(1)	-1.735661(0)	3.074329(-2)	-2.325326(-4)
13	2.492372(5)	-9.351094(4)	1.497706(4)	-1.327578(3)	7.034002(1)	-2.227787(0)	3.905472(-2)	-2.923659(-4)
14	1.554055(5)	-5.847188(4)	9.393681(3)	-8.354542(2)	4.442797(1)	-1.412750(0)	2.487460(-2)	-1.870930(-4)

\*Numeral A(k) should read as  $A \times 10^k$ .

TABLE 9.- COMPARISON AMONG VARIOUS METHODS OF MEMORY SIZES NECESSARY FOR STORING THE COEFFICIENTS AND THE COMPUTATION TIME; THE LATTER IS SHOWN AS THE RATIO TO THE TIME IN S0(2)

Method	Hudson and Mahle (ref. 2)	Kockarts (ref. 3)			S0(1)	S0(2)
Division	Band-to-band	Band-to-band	10 Å	500 cm <sup>-1</sup>	Band-to-band	50 Å
Memory size	5538	320	480	256	304	96
Computation time	~3.3 <sup>a</sup>	~3.7	~5	~3	~3	1

<sup>a</sup>Needs additional time for calculating the necessary coefficients by interpolation.

TABLE 10.- PERCENTAGE DIFFERENCE OF THE RESULT CALCULATED BY METHOD SO(2)  
FROM THAT BY HUDSON-MAHLE ORIGINAL METHOD

Molecule	Temperature, °K	O <sub>2</sub> column density, cm <sup>-2</sup>					
		10 <sup>18</sup>	10 <sup>19</sup>	10 <sup>20</sup>	10 <sup>21</sup>	10 <sup>22</sup>	10 <sup>23</sup>
		%	%	%	%	%	%
O <sub>2</sub>	300	21.5	28.7	23.2	2.4	2.9	-2.7
	250	17.9	19.8	12.3	-2.5	1.3	-3.7
	200	13.0	11.5	4.3	-8.7	-3.4	10.5
	150	7.1	4.0	-3.1	-12.8	-2.4	12.8
	V.T.*	14.0	9.8	7.0	-6.0	-0.5	8.0
N <sub>2</sub> O	300	-0.4	2.4	-0.3	-8.2	-4.0	-19.6
	250	-0.1	2.8	1.4	-3.3	6.0	-6.2
	200	-0.8	1.7	5.6	0.8	9.2	14.3
	150	0.3	3.5	4.5	4.8	20.1	10.6
	V.T.	-1.6	2.2	6.2	-5.1	0.6	9.8
HNO <sub>3</sub>	300	-0.7	2.5	0.5	-7.6	-3.4	-19.0
	250	-0.4	2.8	1.9	-3.3	5.9	-6.0
	200	-1.1	1.6	6.0	0.1	8.3	13.9
	150	-0.1	3.4	4.5	3.5	18.6	9.9
	V.T.	-1.9	2.0	6.6	-4.9	0.5	9.5
HCl	300	1.3	1.8	-4.4	-10.8	-7.2	-22.9
	250	1.6	2.9	-1.0	-2.8	5.8	-8.4
	200	1.4	3.1	4.2	4.6	13.3	12.7
	150	2.3	5.0	5.9	12.4	26.4	11.9
	V.T.	0.6	3.9	4.7	-5.2	1.0	8.0
SO <sub>2</sub>	300	-2.9	1.6	1.1	-8.1	-3.4	-16.5
	250	-2.7	1.6	1.8	-5.0	4.1	-5.4
	200	-3.6	-0.1	5.5	-2.6	4.8	12.2
	150	-2.5	1.8	3.1	-0.5	13.9	7.3
	V.T.	-4.3	0.2	6.1	-6.3	-1.3	8.5
H <sub>2</sub> O	300	21.8	20.2	9.2	-0.3	-12.3	-42.6
	250	22.2	24.5	19.3	26.6	21.9	14.9
	200	22.5	27.7	30.1	59.4	63.9	22.4
	150	23.4	31.6	43.4	98.4	112.2	43.9
	V.T.	22.0	29.2	29.4	23.6	18.1	9.2
H <sub>2</sub> O <sub>2</sub>	300	-2.4	0.5	-1.5	-9.2	-3.6	-15.7
	250	-2.2	0.9	-0.0	-5.4	3.5	-5.3
	200	-2.9	-0.2	4.2	-2.1	4.1	11.4
	150	-1.8	1.8	2.9	1.1	13.3	6.1
	V.T.	-3.6	0.3	4.6	-6.7	-1.9	8.2

TABLE 10.- PERCENTAGE DIFFERENCE OF THE RESULT CALCULATED BY METHOD SO(2)  
FROM THAT BY HUDSON-MAHLE ORIGINAL METHOD — CONCLUDED

Molecule	Temperature, °K	O <sub>2</sub> column density, cm <sup>-2</sup>					
		10 <sup>18</sup>	10 <sup>19</sup>	10 <sup>20</sup>	10 <sup>21</sup>	10 <sup>22</sup>	10 <sup>23</sup>
		%	%	%	%	%	%
CO <sub>2</sub>	300	5.0	6.3	-2.8	-12.3	-12.2	-28.0
	250	5.3	9.2	4.4	3.1	6.1	13.2
	200	5.1	11.4	12.6	19.7	22.6	8.6
	150	6.4	14.3	20.7	38.9	42.7	9.8
	V.T.	4.9	12.6	12.4	0.0	2.2	2.9
CFC1 <sub>3</sub>	300	-5.3	-3.7	-7.4	-12.3	-4.6	-18.3
	250	-5.0	-3.1	-5.2	-7.1	5.0	-5.8
	200	-5.4	-3.7	-0.9	-2.4	8.1	13.7
	150	-4.5	-2.0	-1.1	2.3	18.7	9.9
	V.T.	-6.1	-3.2	-0.4	-8.7	-0.3	9.4
CF <sub>2</sub> Cl <sub>2</sub>	300	-0.1	3.1	0.3	-8.9	-7.0	-23.9
	250	0.2	3.3	2.0	-2.9	5.9	-8.4
	200	-0.5	2.4	6.0	1.9	12.9	14.6
	150	0.6	3.9	5.0	6.8	25.4	13.6
	V.T.	-1.5	2.9	6.8	-5.2	1.1	8.9

<sup>a</sup>V.T. (variable temperature) indicates the height-dependent temperature.



5  
2  
7



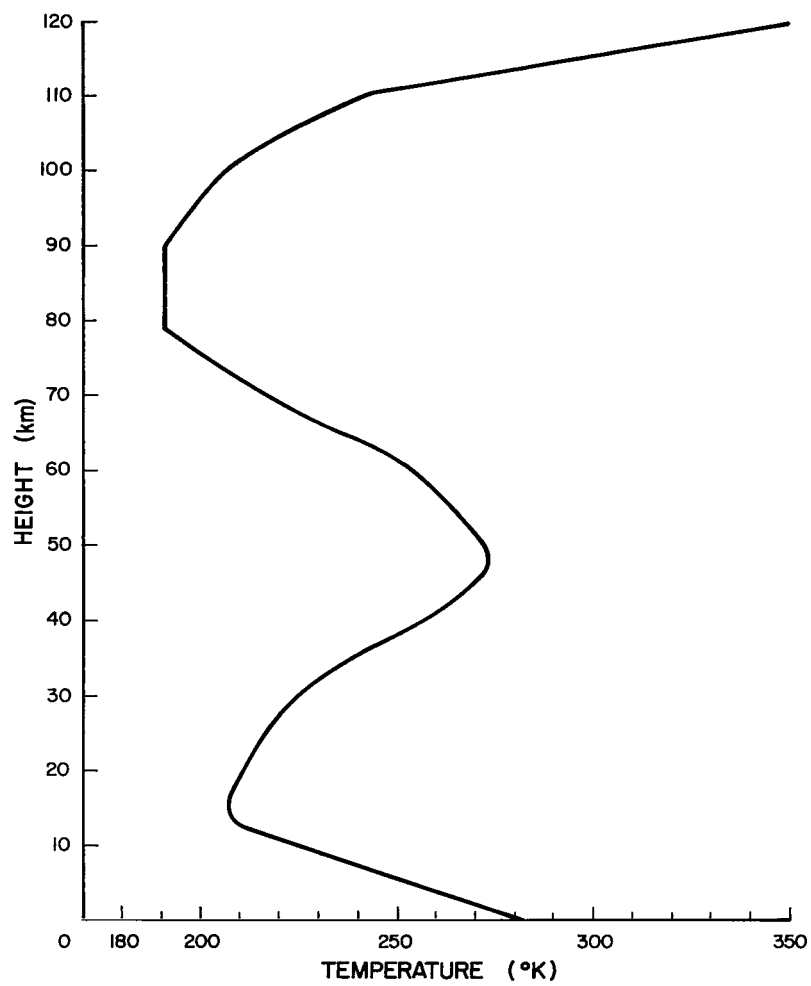


Figure 1.- The temperature profile used in the model calculations.

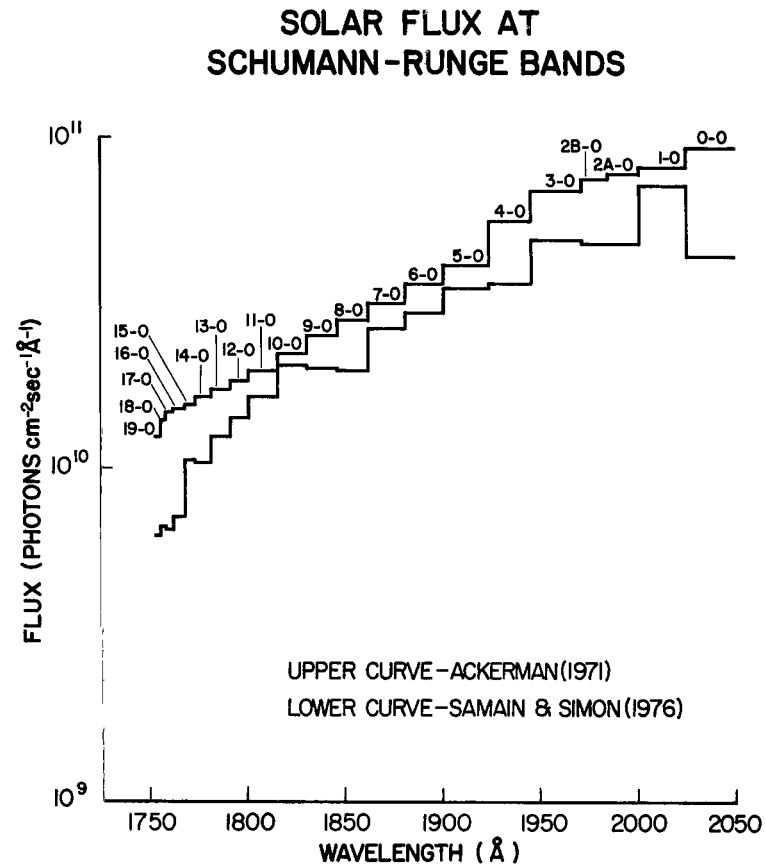


Figure 2.- Solar fluxes at each band of the Schumann-Runge band region.

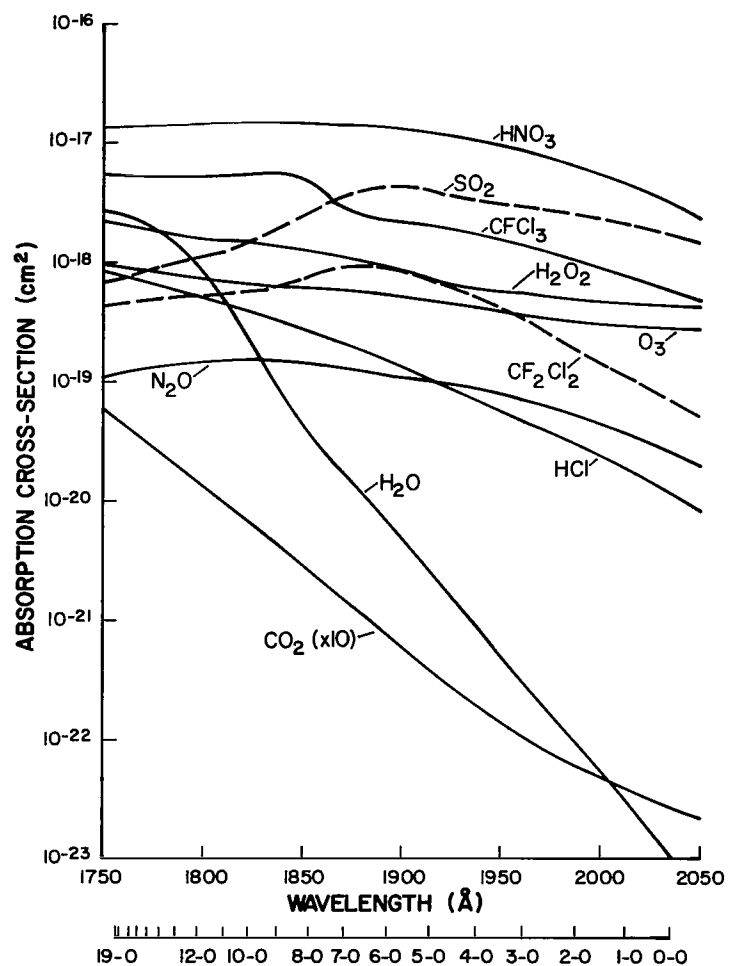


Figure 3.- Absorption cross sections of various molecules in the Schumann-Runge band system.

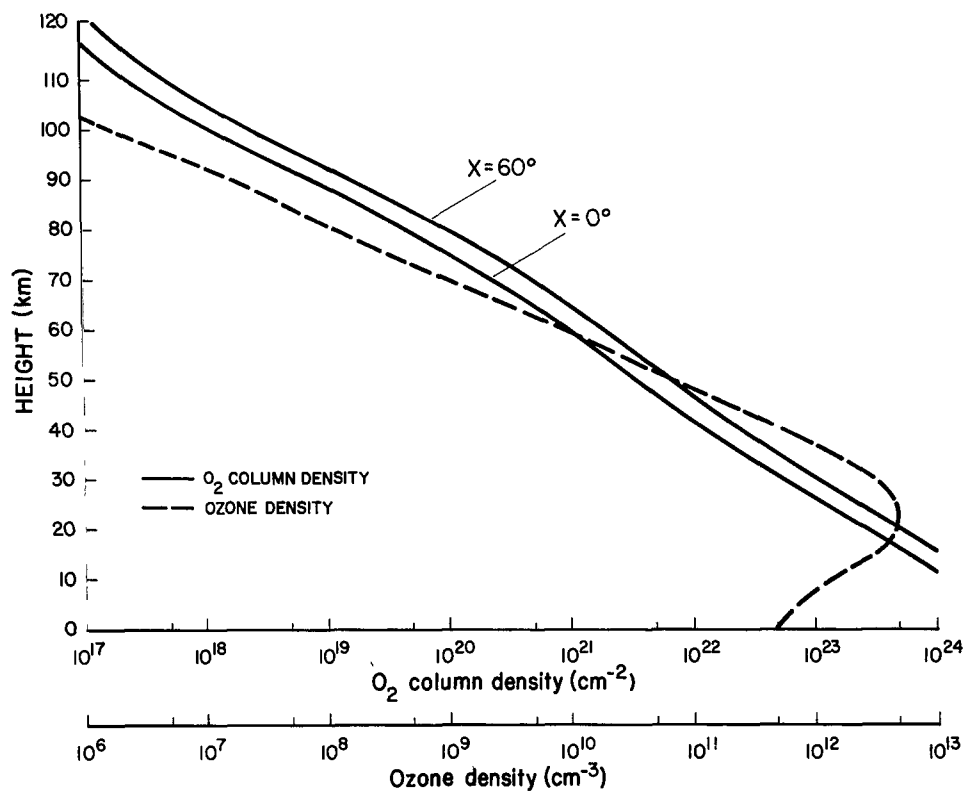
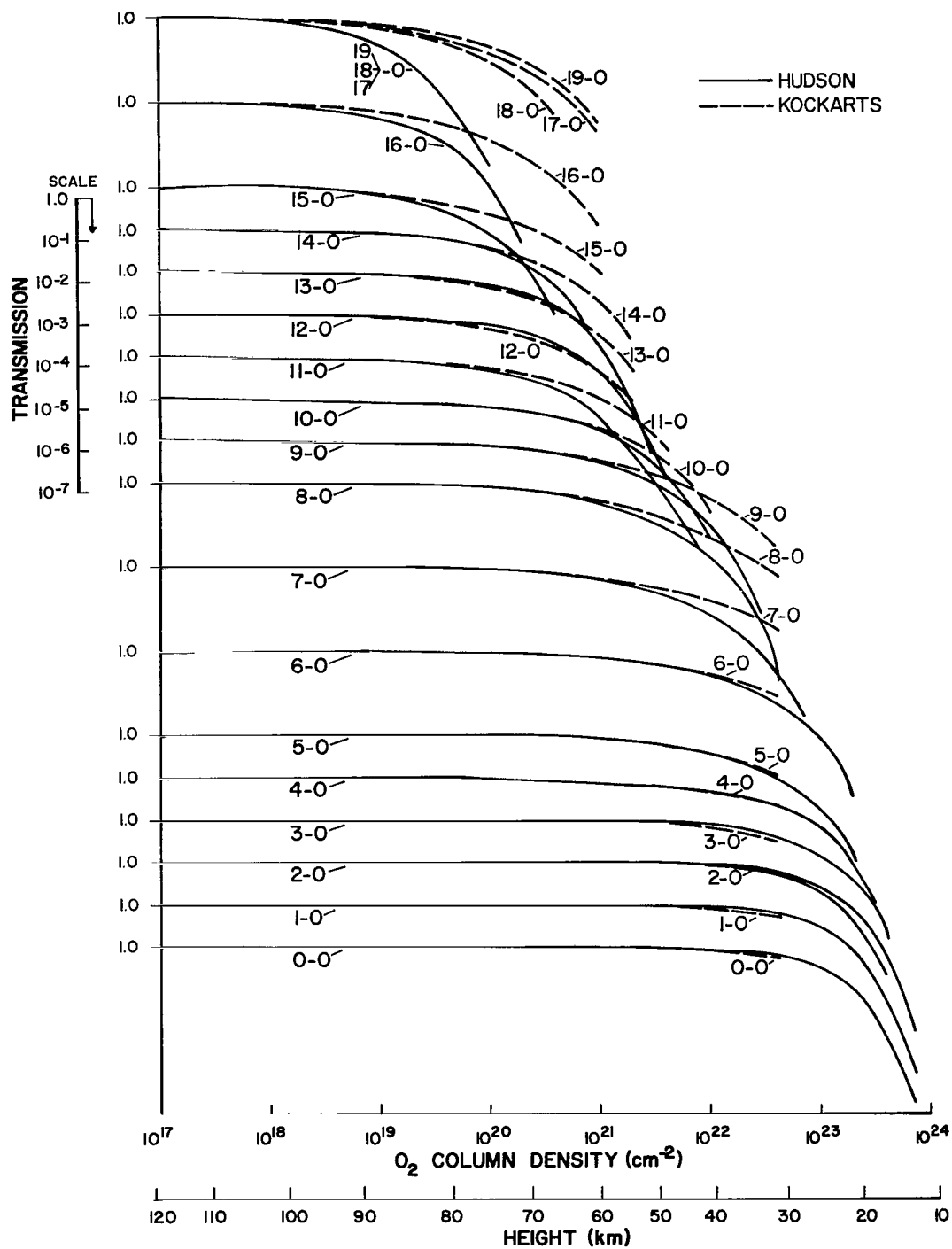
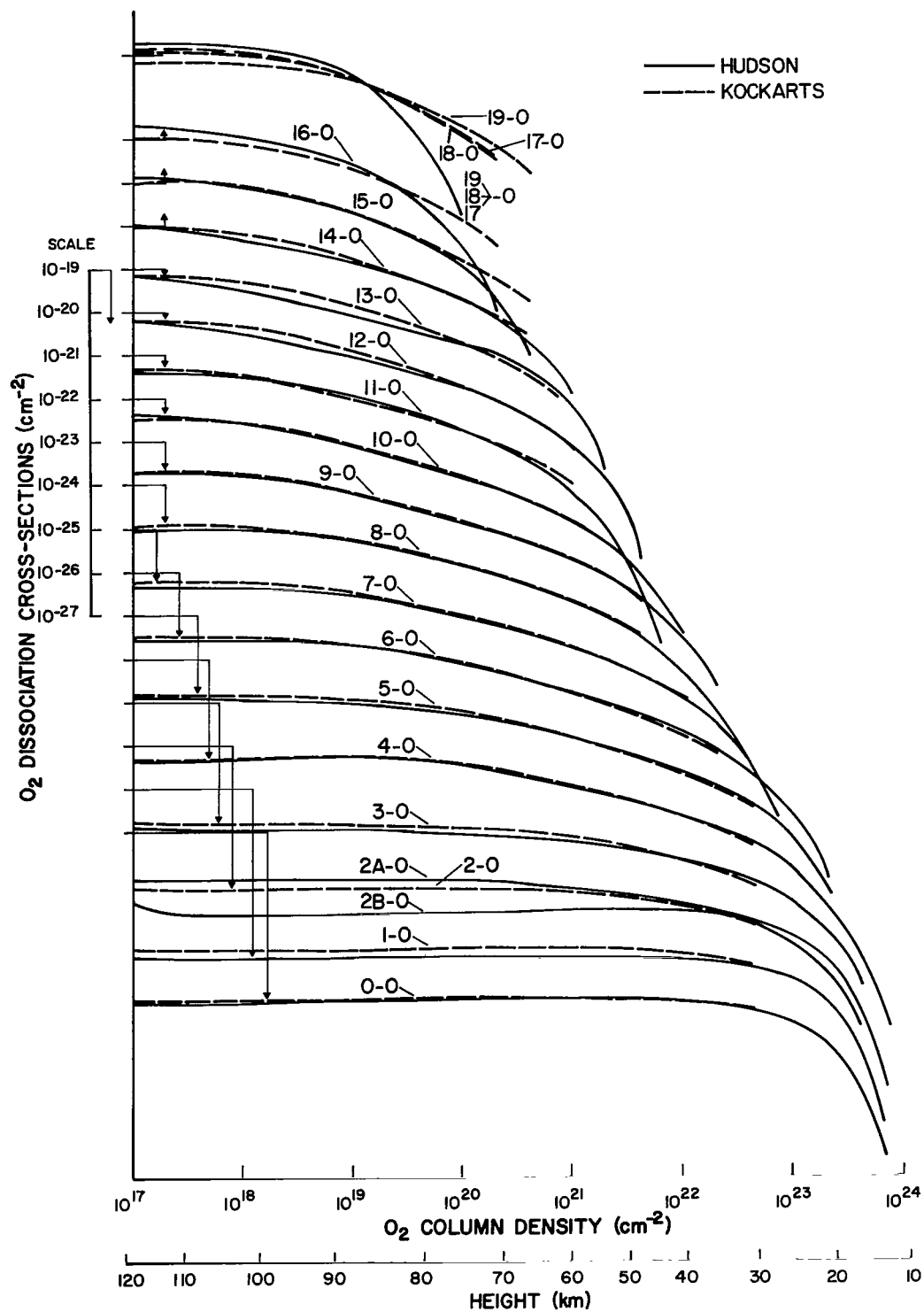


Figure 4.- An ozone density profile based on observations, and the relationship between the  $O_2$  column density and the height of the atmosphere for the condition of overhead sun and a  $60^\circ$  solar incidence angle.



(a) Transmission at each band of the Schumann-Runge system.

Figure 5.- Comparison between the Hudson-Mahle and Kockarts methods.



(b)  $O_2$  predissociation coefficients at each Schumann-Runge band.

Figure 5.- Concluded.

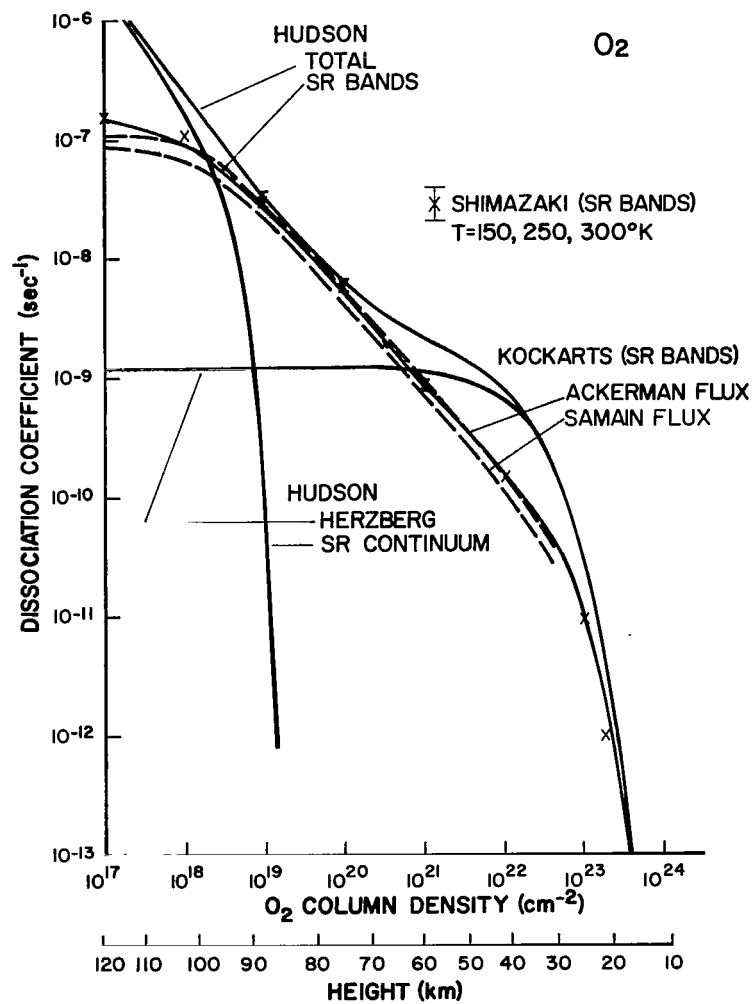


Figure 6.- Comparison of the  $O_2$  dissociation coefficients calculated by various methods.

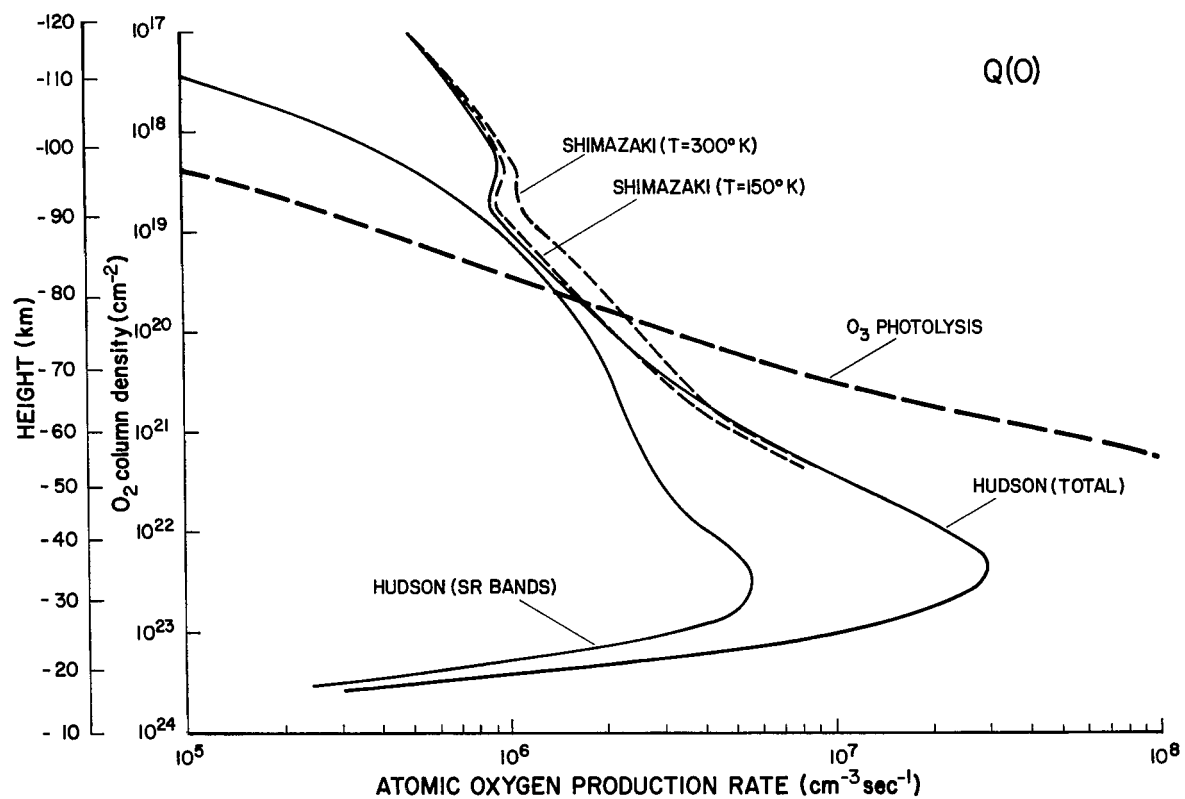
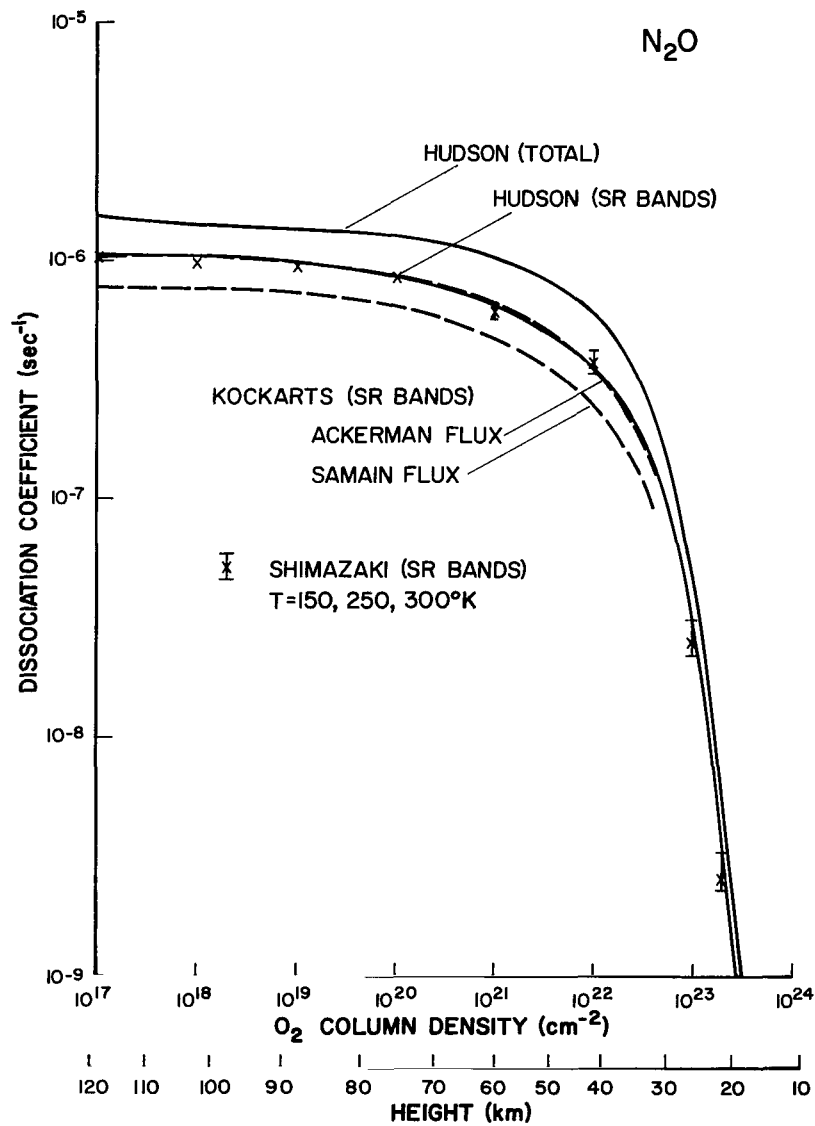


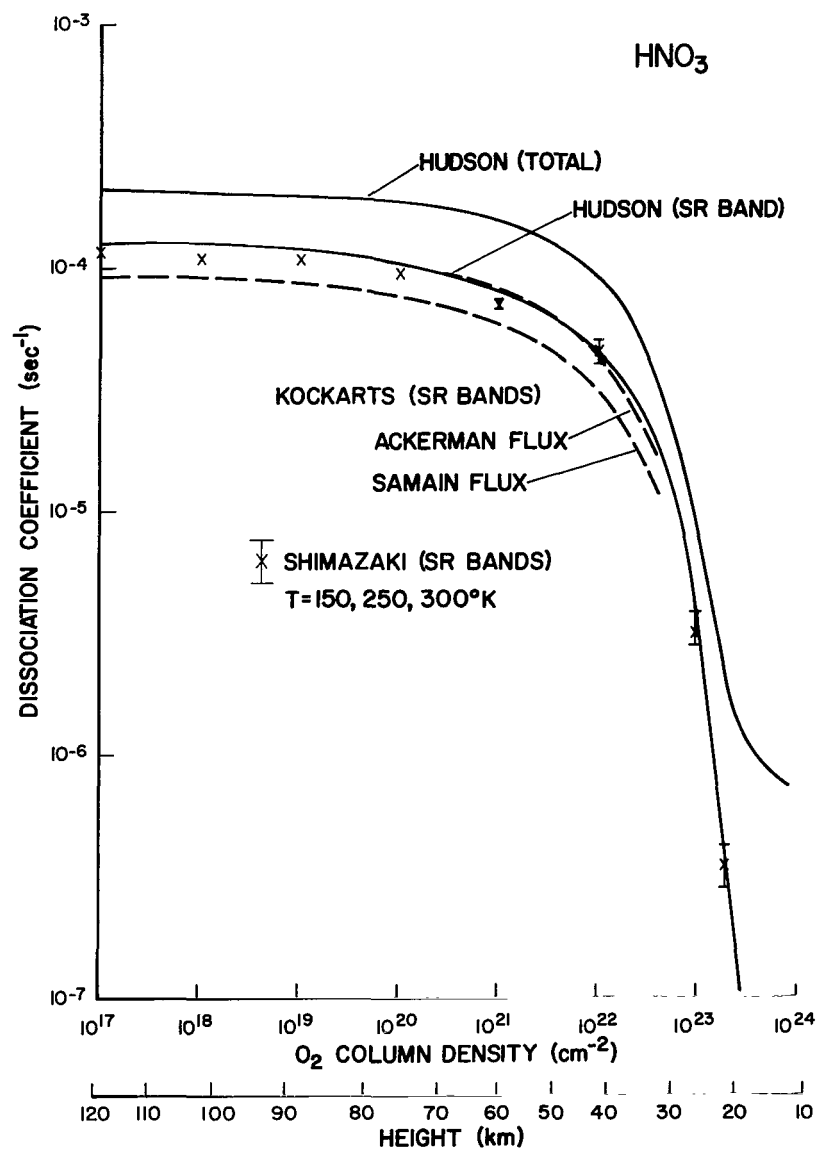
Figure 7.- Profiles of atomic oxygen production rate by  $O_2$  and  $O_3$  photolyses calculated by the Hudson-Mahle method and the Shimazaki-Ogawa method.





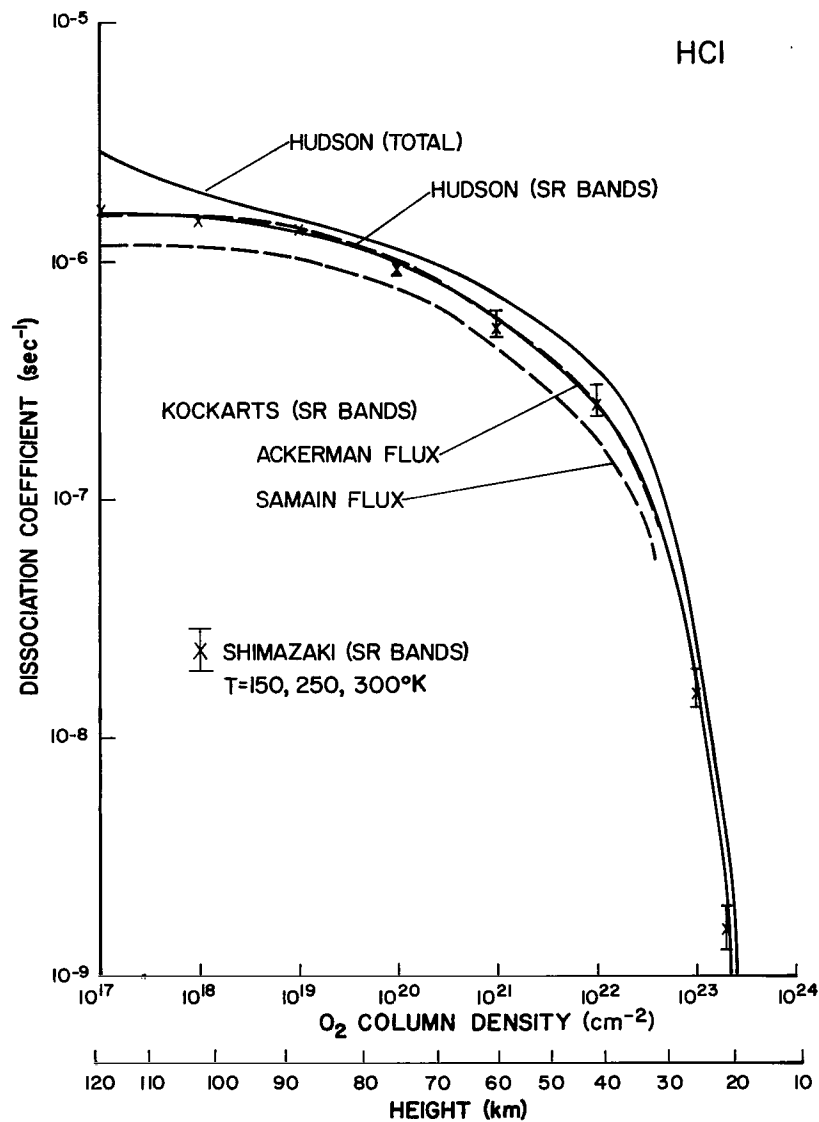
(a) Dissociation coefficient for  $N_2O$ .

Figure 8.- Comparison of the dissociation coefficients calculated by various methods.



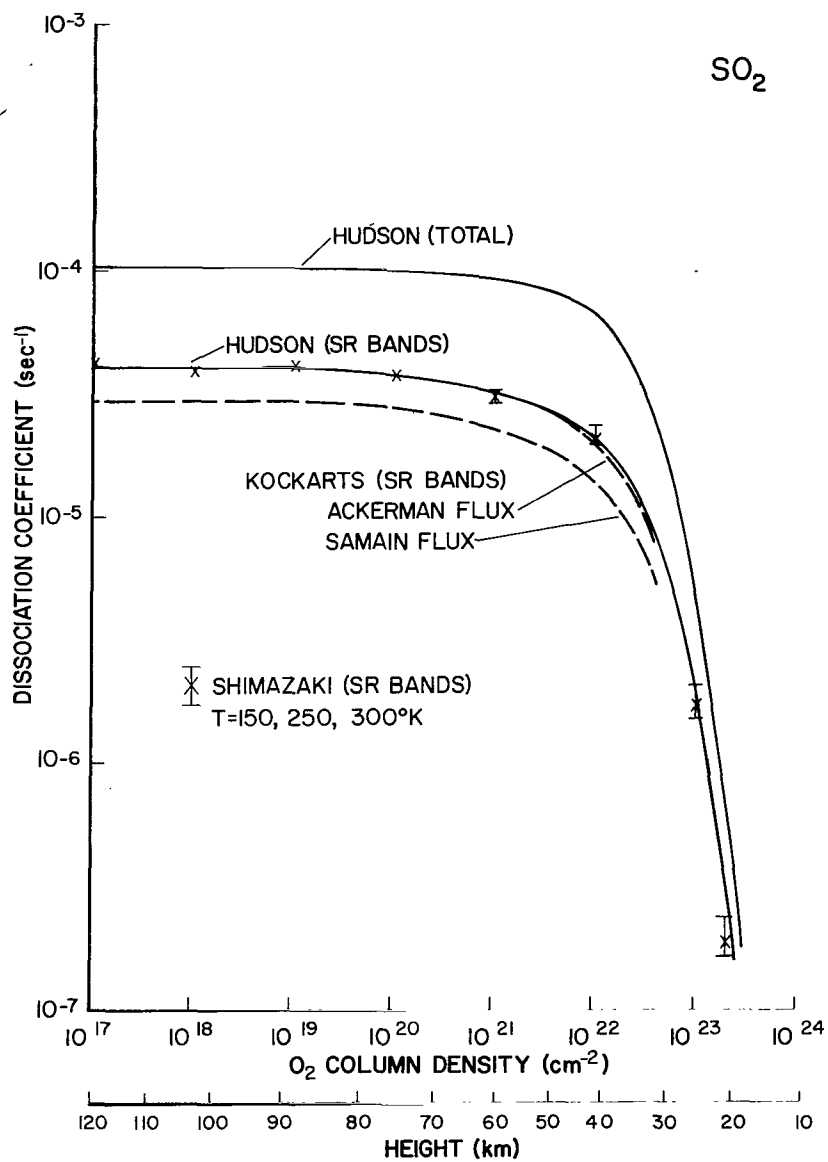
(b) Dissociation coefficient for  $\text{HNO}_3$ .

Figure 8.- Continued.



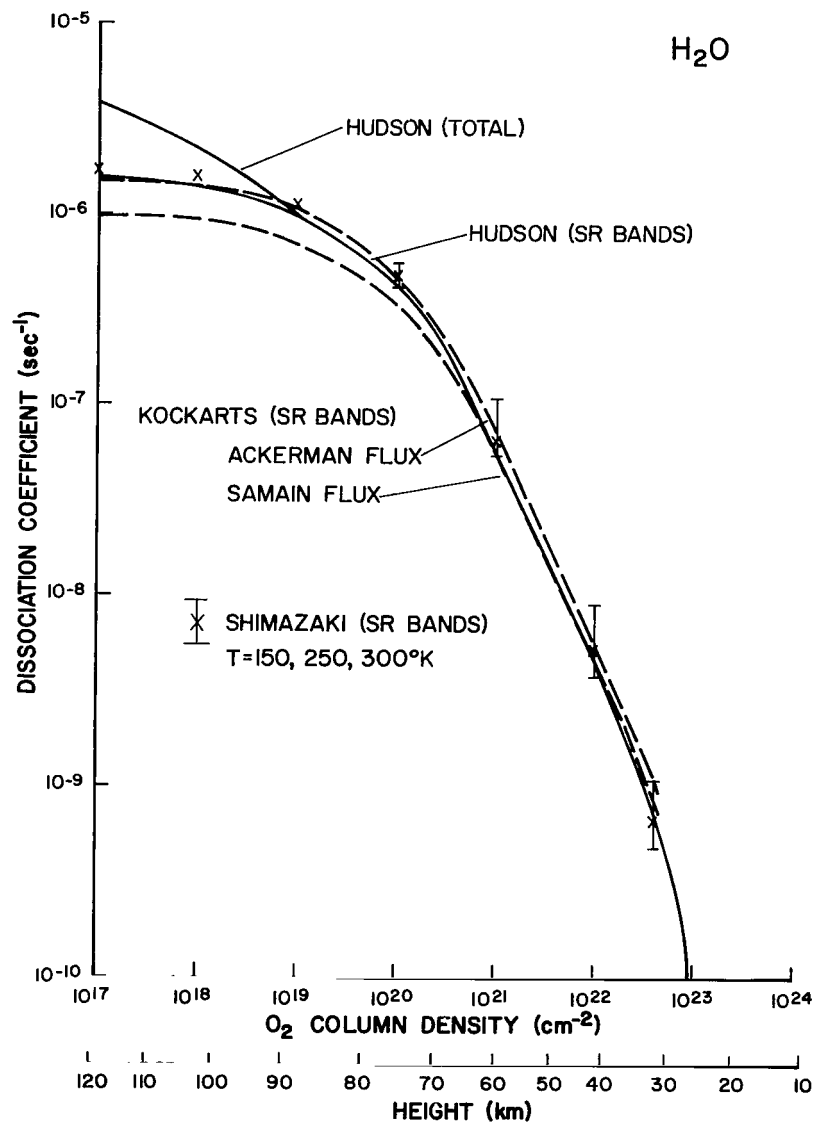
(c) Dissociation coefficient for HCl.

Figure 8.- Continued.



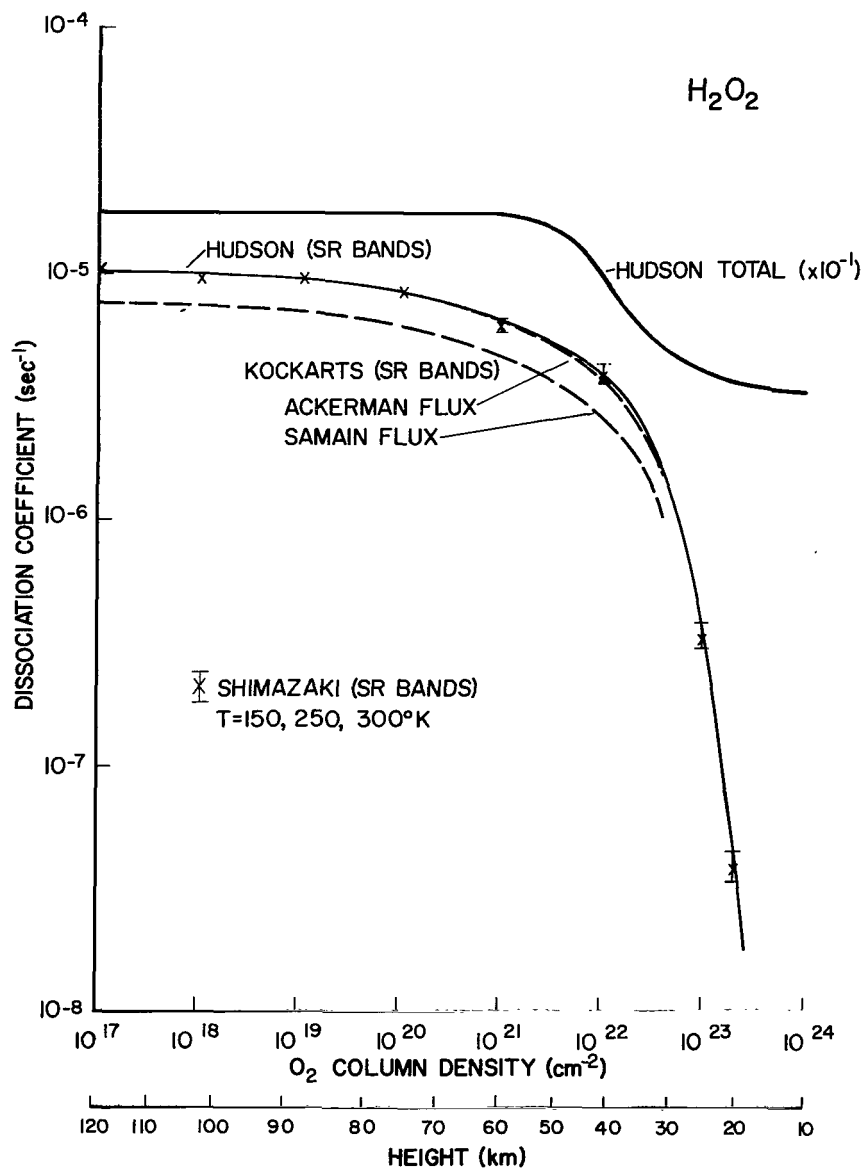
(d) Dissociation coefficient for  $\text{SO}_2$ .

Figure 8.- Continued.



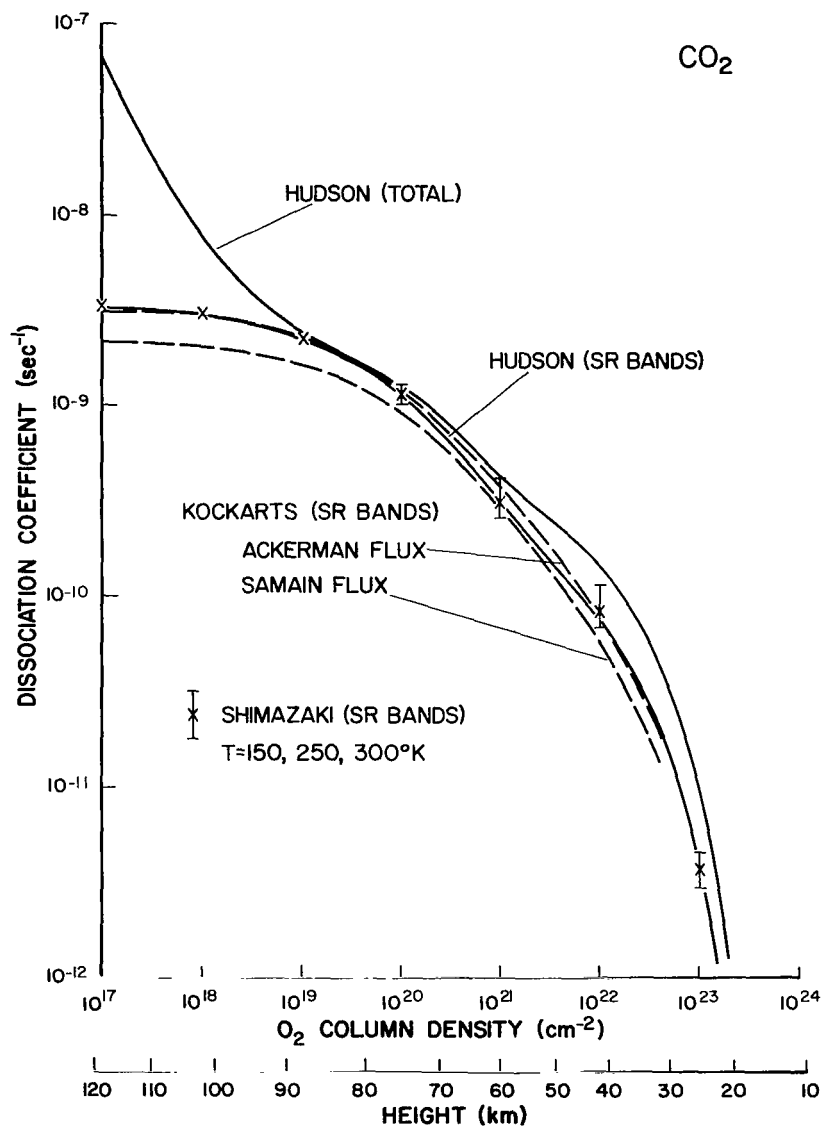
(e) Dissociation coefficient for  $H_2O$ .

Figure 8.- Continued.



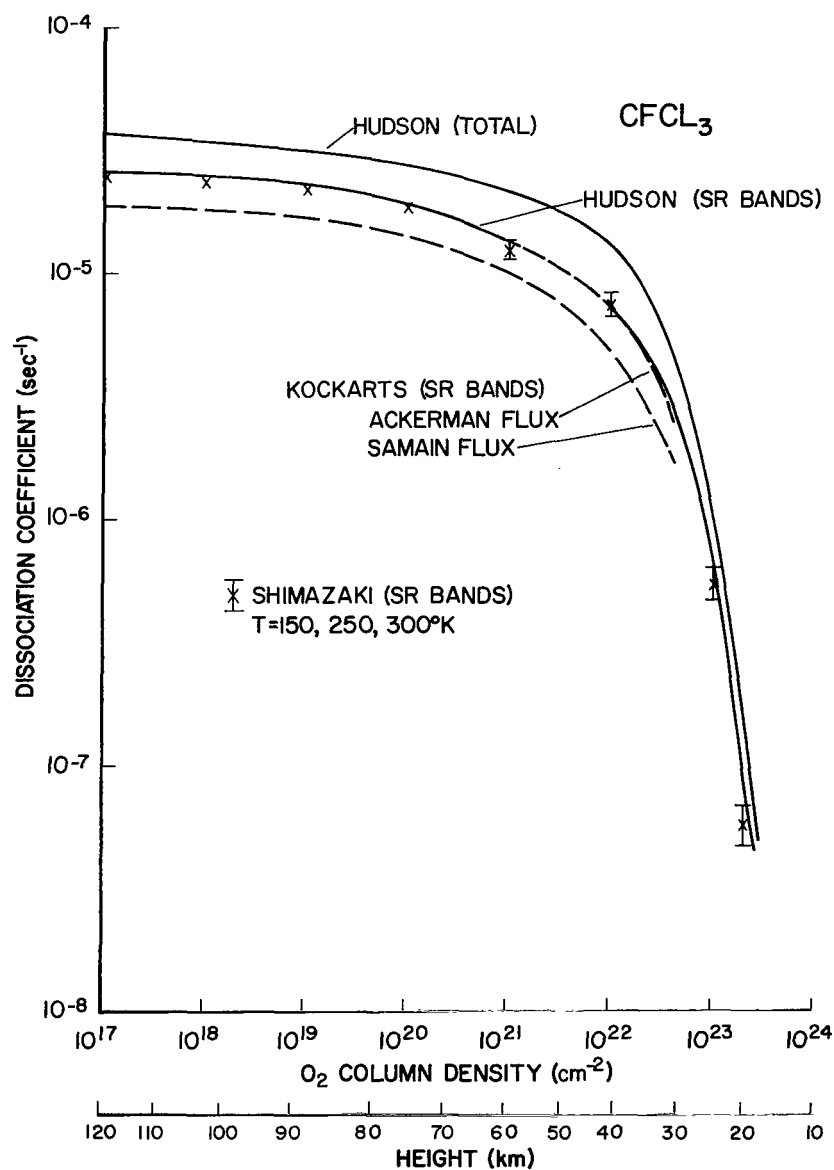
(f) Dissociation coefficient for  $H_2O_2$ .

Figure 8.- Continued.



(g) Dissociation coefficient for  $\text{CO}_2$ .

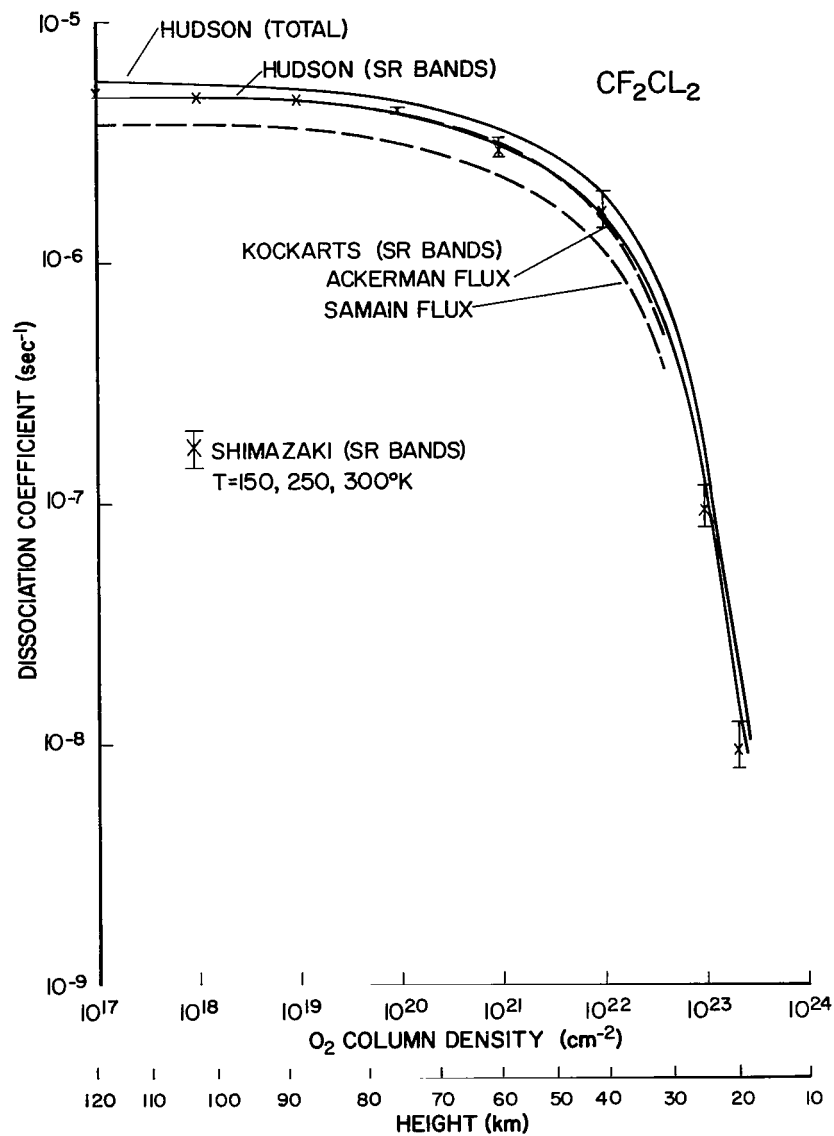
Figure 8.- Continued.



(h) Dissociation coefficient for CFCl<sub>3</sub>.

Figure 8.- Continued.





(i) Dissociation coefficient for CF<sub>2</sub>Cl<sub>2</sub>.

Figure 8.- Concluded.



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